

# SEARCH REQUEST FORM

Patent and Trademark Office

Requestor's

Name:

BERCH

Serial

Number:

03/26508

Date:

3/10/04

Phone:

571-272-0663

Art Unit:

1624

Office

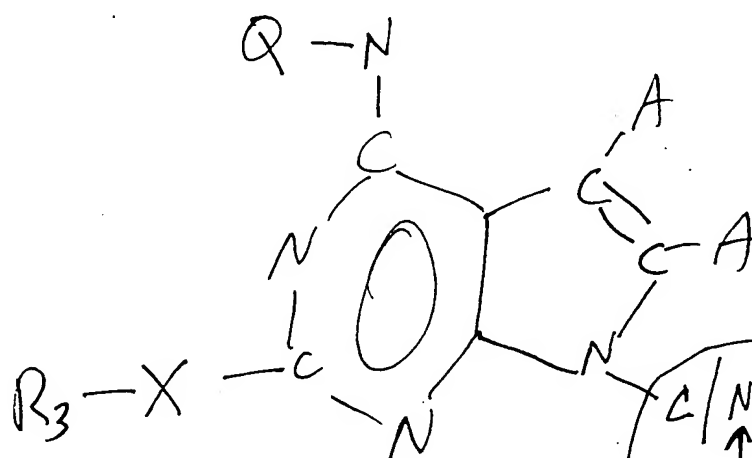
Room 5C01

Mailbox

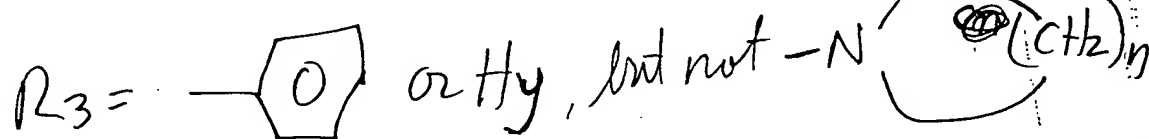
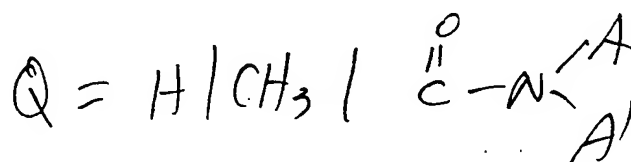
5C18

## Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevant citations, authors, keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevant claim(s).



A, A' = H/CH<sub>3</sub>:



X = O/N/S/bond

n = 3-8

~~If you get zero hits, let this be A~~

STAFF USE ONLY

Date completed:

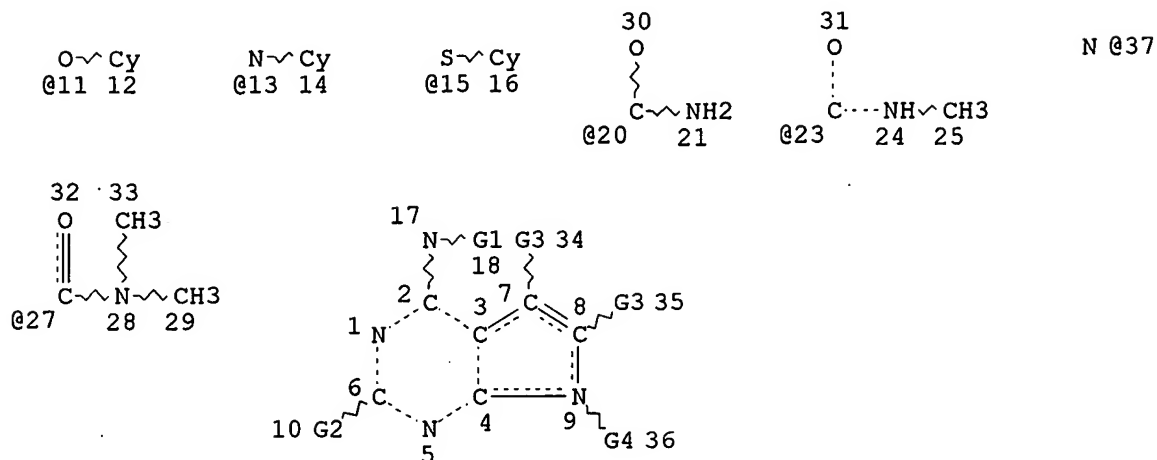
Searcher's

PCT/26508

(FILE 'REGISTRY' ENTERED AT 14:26:01 ON 12 MAR 2004)

L1

STR



VAR G1=H/CH3/20/23/27

VAR G2=11/13/15/CY

VAR G3=H/CH3

VAR G4=C/37/H

NODE ATTRIBUTES:

NSPEC IS R AT 37

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L2 249 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 12153 ITERATIONS

249 ANSWERS

SEARCH TIME: 00.00.01

=> d scan

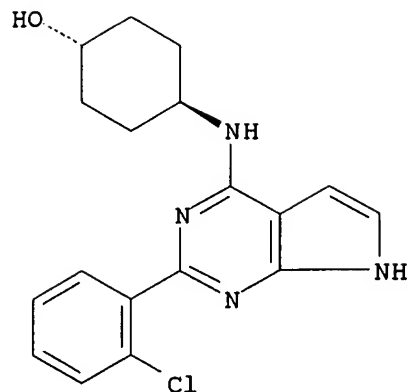
L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Cyclohexanol, 4-[2-(2-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI)

MF C18 H19 Cl N4 O

Relative stereochemistry.

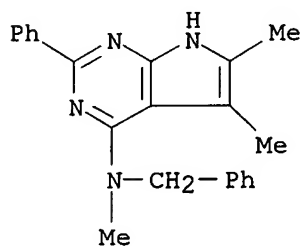
PCT/26508



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

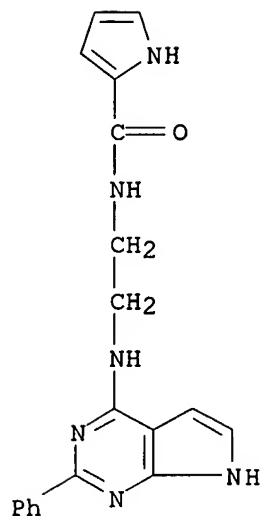
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 1H-Pyrrolo[2,3-d]pyrimidin-4-amine, N,5,6-trimethyl-2-phenyl-N-(phenylmethyl)- (9CI)  
MF C22 H22 N4



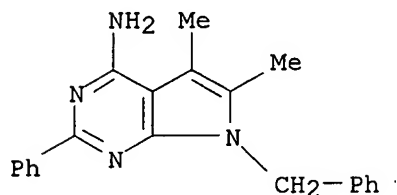
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 1H-Pyrrolo[2,3-d]pyrimidin-4-amine, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI)  
MF C19 H18 N6 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-  
 (phenylmethyl)- (9CI)  
 MF C21 H20 N4

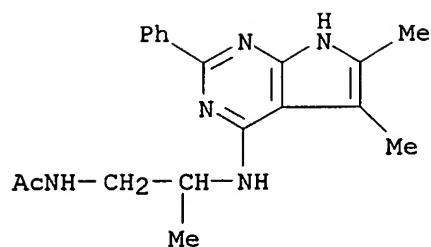


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
 IN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-  
 yl)amino]propyl]- (9CI)  
 MF C19 H23 N5 O

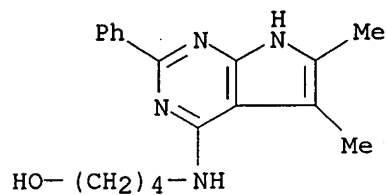


PCT/26508



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 1-Butanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]- (9CI)  
MF C18 H22 N4 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

FILE 'HCAPLUS' ENTERED AT 14:29:08 ON 12 MAR 2004  
L3 30 S L2

=> sel hit l3 1-30 rn  
E1 THROUGH E245 ASSIGNED

FILE 'HOME' ENTERED AT 14:29:20 ON 12 MAR 2004

E0490133

2004 077 14:27:27

REQUEST NUMBER: P077138C

File Reg. @ 249 ans.

10525478

BEVERLY SHEARS  
US PATENT & TRADEMARK OFFICE  
BIOTECH/CHEM LIBRARY, RM 1A54  
HENRY REMSEN, JR. BLDG.  
400 DULANY ST.  
ALEXANDRIA, VA 22314

## CHEMICAL ABSTRACTS "REGISTRY FILE"

The REGISTRY File contains chemical substance records for substances identified by the CAS Registry System. The codes used to label the fields are shown below.

### SUBSTANCE INFORMATION FIELD CODES

AF	Alternate Molecular Formula
AR	Alternate CAS Registry Number
CCI	Component Class Identifier
CCN	Condensed Chemical Name (all names)
CI	Class Identifier
CIL	Component Isotope at Unknown Location
CMF	Component Molecular Formula
CN	Chemical Name (up to 50)
COMP	Composition
CRN	Component CAS Registry Number
DEF	Definition
DR	Deleted CAS Registry Number
ENTE	Editor Note
FCN	All Chemical Names
FS	File Segment
IL	Isotope at Unknown Location
IN	CA Index Name
LC	CAS Registry Number Locator
MF	Molecular Formula
PCT	Polymer Class Term
PR	Preferred CAS Registry Number
REF	Number of References in CAPIUS, CA, and CAOLD, and the number of references in CA for the non-specific derivatives
RN	CAS Registry Number
RR	Replacing Registry Number
RSD	Ring System Data
SCN	Short Chemical Name (IN and OTHER NAMES)
SR	Source of Registration
SRSD	Short Ring System Data
STR	Structure Diagram with stereo bond and R/S/Z/E designations, if available

STF Flat Structure Diagram (no stereo bonds)  
 STS Structure Diagram with stereo bonds, if available

Sequence Field Codes:

NA Nucleic Acid  
 NTE Note  
 PNTE Patent Annotation  
 SEQ Sequence (1-letter amino acid codes)  
 SEQ3 Sequence (3-letter amino acid codes)  
 SQL Sequence Length

Property Field Codes:

BCF Bioconcentration Factor  
 BP Boiling Point  
 DEN Density  
 ECND Electric Conductivity  
 ECON Electric Conductance  
 ERES Electric Resistance  
 EREST Electric Resistivity  
 FP Flash Point  
 FRB Freely Rotable Bonds  
 HAC H acceptors  
 HD H donors  
 HVAP Enthalpy of Vaporization  
 KOC Organic Carbon Adsorption Coefficient  
 LD50 Median Lethal Dose  
 LOGD logD  
 LOGP logP  
 MM Magnetic Moment  
 MP Melting Point  
 MW Molecular Weight  
 ORP Optical Rotatory Power  
 PKA pKa  
 RI Refractive Index  
 SLB.MOL Molar Solubility  
 TG Glass Transition Temperature  
 TS Tensile Strength  
 VP Vapor Pressure

## CA DOCUMENT REFERENCE FIELD CODES

AN	Accession Number
TI	Title of Document
AU	Author
IN	Patent Inventor
CS	Corporate Source
PA	Patent Assignee
SO	Source
PB	Publisher
PUI	Publisher Item Identifier
URL	Uniform Resource Locator
DT	Document Type
LA	Language
IC	International Patent Classification (IPC)
ICM	Main IPC
ICS	Secondary IPC
ICA	Additional or Supplementary IPC
ICI	Index or Complementary IPC
NCL	National Patent Classification Code
CC	Classification Code (CA Section Code and Title and CA Section Cross-Reference Code)
FAN.CNT	Family Accession Number Count
CY.CNT	Patent Country Count
PN.CNT	Patent Number Count
PI	Patent Information or Patent Family Table
DS	Designated States (patent)
AI	Patent Application Information
PRAI	Priority Application Information
PY	Publication Year
FAN	Family Accession Number
OS	Other Source
GI	Graphic Image
AB	Abstract
ST	Supplementary Term (CA Keywords)
IT	Index Term
RL	Role
REC.CNT	Cited References Count
RE	Cited References
RETABLE	Cited References Table

# STN INTERNATIONAL®

REGISTRY FILE SEARCH STATISTICS - P077138C

17 MAR 2004 20:03:16 PAGE

4

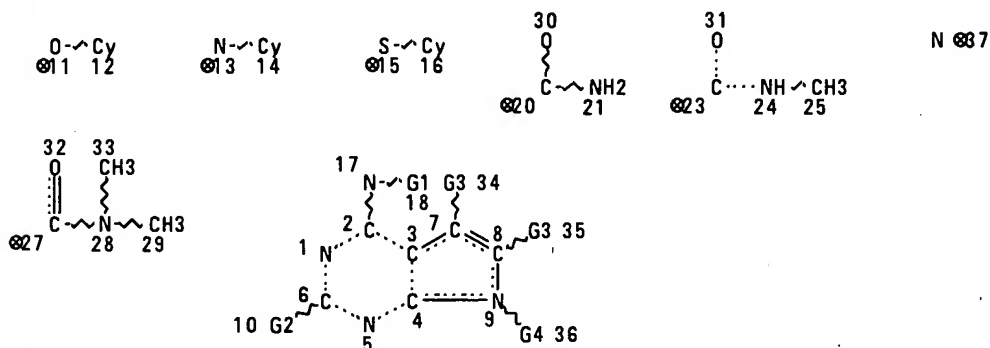
249 ANSWERS PRINTED IN FORMAT 'IDE CAN'

IN FILE 'REGISTRY'

USING QUERY:

L1

STR



VAR G1=H/CH3/20/23/27

VAR G2=11/13/15/CY

VAR G3=H/CH3

VAR G4=C/37/H

NODE ATTRIBUTES:

NSPEC IS R AT 37

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L2 249 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 12153 ITERATIONS

249 ANSWERS

SEARCH TIME: 00.00.01

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

5

L2 ANSWER 1 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 565234-92-6 REGISTRY

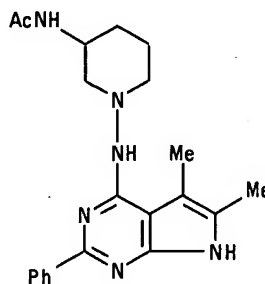
CN Acetamide, *N*-[1-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-3-piperidiny]- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>26</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18 PAGE

6

L2 ANSWER 2 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 553634-53-0 REGISTRY

CN Acetamide,

*N*-[2-[[[6-methyl-7-[2-oxo-2-[4-(3-phenyl-2-propenyl)-1-piperazinyl]ethyl]-2-phenyl-7*H*-pyrrolo[2,3-*d*]-pyrimidin-4-yl]amino]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

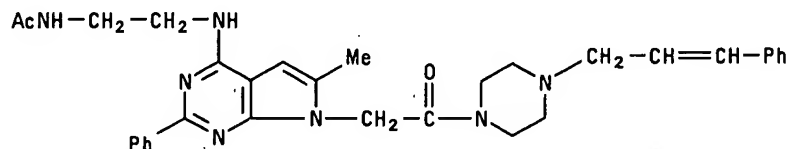
CN *N*-[2-[[[6-Methyl-7-[2-oxo-2-[4-(3-phenylallyl)piperazin-1-yl]ethyl]-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]ethyl]acetamide

FS 3D CONCORD

MF C<sub>32</sub>H<sub>37</sub>N<sub>7</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:85365

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 7

L2 ANSWER 3 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-91-7 REGISTRY

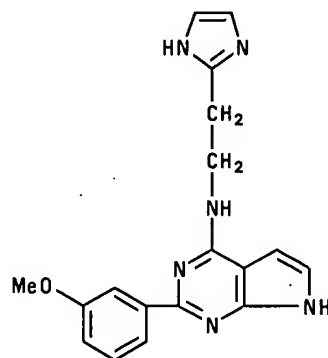
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-[2-(1*H*-imidazol-2-yl)ethyl]-2-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>18</sub>H<sub>18</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

8

L2 ANSWER 4 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-87-1 REGISTRY

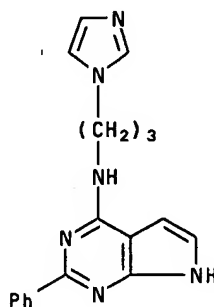
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-[3-(1*H*-imidazol-1-yl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>18</sub>H<sub>18</sub>N<sub>6</sub>

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*

L2 ANSWER 5 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-85-9 REGISTRY

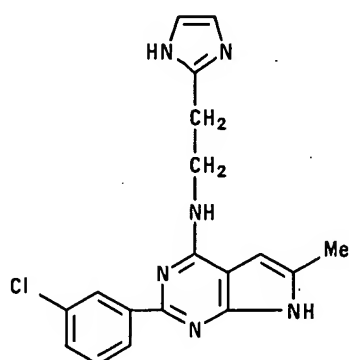
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(3-chlorophenyl)-*N*-[2-(1*H*-imidazol-2-yl)ethyl]-6-methyl- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>18</sub>H<sub>17</sub>ClN<sub>6</sub>

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

10

L2 ANSWER 6 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-83-7 REGISTRY

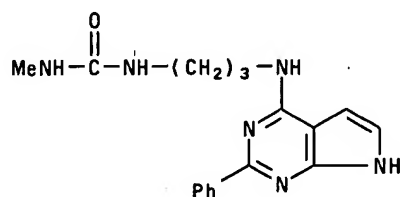
CN Urea, *N*-methyl-*N'*-[3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>17</sub>H<sub>20</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 11

L2 ANSWER 7 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-80-4 REGISTRY

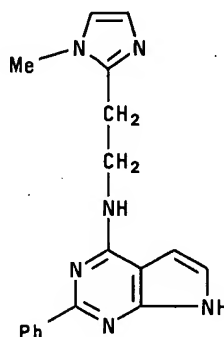
CN 1*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, *N*-[2-(1-methyl-1*H*-imidazol-2-yl)ethyl]-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>18</sub>H<sub>18</sub>N<sub>6</sub>

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

12

L2 ANSWER 8 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-77-9 REGISTRY

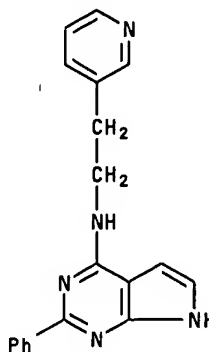
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-phenyl-*N*-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>17</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*

L2 ANSWER 9 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-75-7 REGISTRY

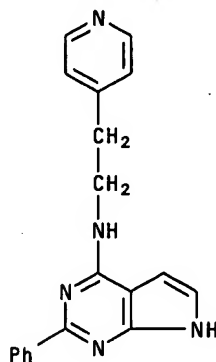
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-phenyl-*N*-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>17</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

14

L2 ANSWER 10 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-73-5 REGISTRY

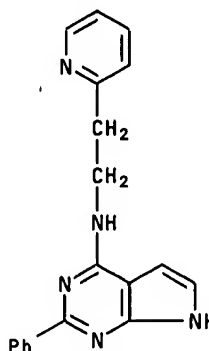
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-phenyl-*N*-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>17</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

15

L2 ANSWER 11 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-71-3 REGISTRY

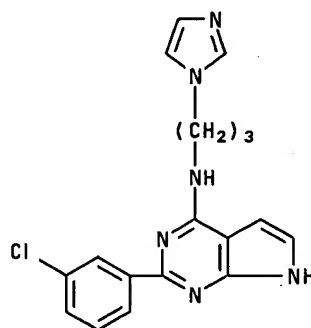
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(3-chlorophenyl)-*N*-[3-(1*H*-imidazol-1-yl)propyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>18</sub>H<sub>17</sub>ClN<sub>6</sub>

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*

L2 ANSWER 12 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-69-9 REGISTRY

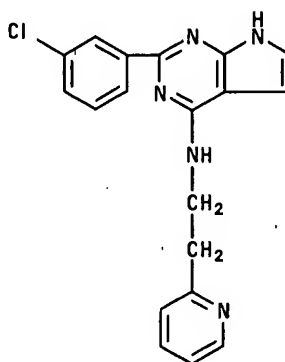
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(3-chlorophenyl)-*N*-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>16</sub>ClN<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*

L2 ANSWER 13 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-67-7 REGISTRY

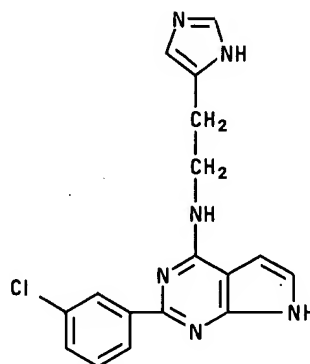
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(3-chlorophenyl)-*N*-[2-(1*H*-imidazol-4-yl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>17</sub>H<sub>15</sub>ClN<sub>6</sub>

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

18

L2 ANSWER 14 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-35-9 REGISTRY

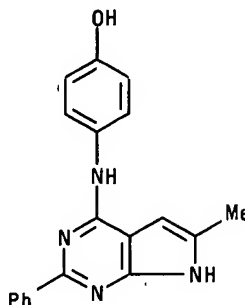
CN Phenol, 4-[(6-methyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>16</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

\*\*\*\*\*

L2 ANSWER 15 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 512848-48-5 REGISTRY

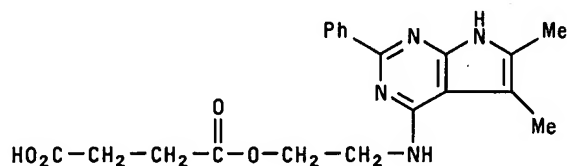
CN Butanedioic acid, mono[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl] ester  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>22</sub>N<sub>4</sub>O<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:321287

\*\*\*\*\*

L2 ANSWER 16 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 512848-47-4 REGISTRY

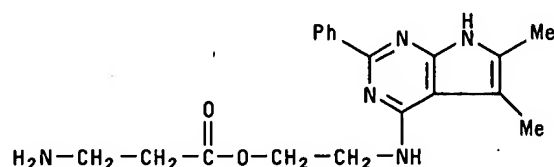
CN  $\beta$ -Alanine, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:321287

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

21

L2 ANSWER 17 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 500736-10-7 REGISTRY

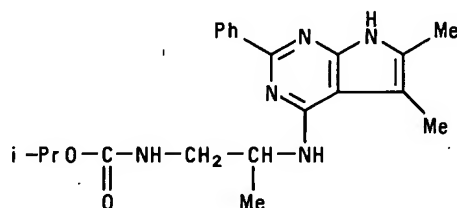
CN Carbamic acid, [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>27</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:221598

\*\*\*\*\*

L2 ANSWER 18 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 500736-09-4 REGISTRY

CN Cyclohexanol,

4-[[2-(3-furanyl)-5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
(9*CI*) (CA INDEX NAME)

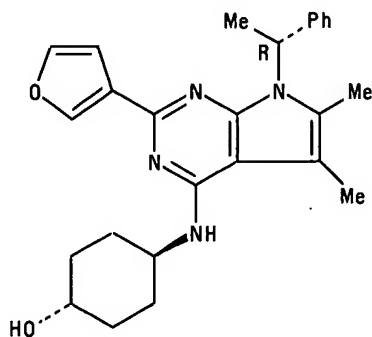
FS STEREOSEARCH

MF C<sub>26</sub>H<sub>30</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:221598

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

23

L2 ANSWER 19 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 500736-03-8 REGISTRY

CN Glycine, (1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*-, trifluoroacetate (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>21</sub>H<sub>25</sub>N<sub>5</sub>O<sub>2</sub>.xC<sub>2</sub>HF<sub>3</sub>O<sub>2</sub>

SR CA

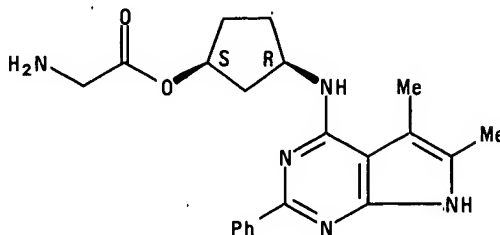
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

CM 1

CRN 251946-51-7

CMF C<sub>21</sub>H<sub>25</sub>N<sub>5</sub>O<sub>2</sub>

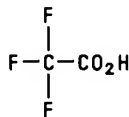
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C<sub>2</sub>HF<sub>3</sub>O<sub>2</sub>



2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:321287

REFERENCE 2:

138:221598

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

24

L2 ANSWER 20 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 500736-02-7 REGISTRY

CN Carbamic acid, [1-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

OTHER NAMES:

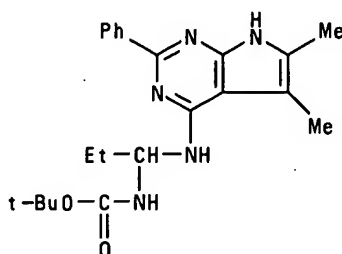
CN 4-[[2-Methyl-1-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>22</sub>H<sub>29</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:221598

\*\*\*\*\*

L2 ANSWER 21 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 476006-54-9 REGISTRY

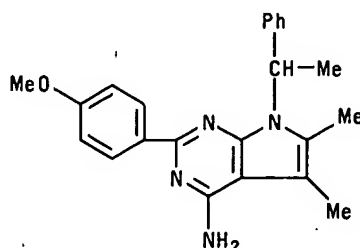
CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(4-methoxyphenyl)-5,6-dimethyl-7-(1-phenylethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>23</sub>H<sub>24</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:379680

\*\*\*\*\*

L2 ANSWER 22 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443760-85-8 REGISTRY

CN Methanesulfonamide,

*N*-[*trans*-4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

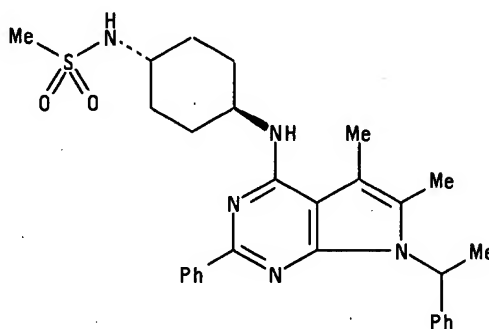
FS STEREOSEARCH

MF C<sub>29</sub>H<sub>35</sub>N<sub>5</sub>O<sub>2</sub>S

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:221598

REFERENCE 2:

137:109485

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

27

L2 ANSWER 23 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443760-84-7 REGISTRY

CN Acetamide,

*N*-[*trans*-4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

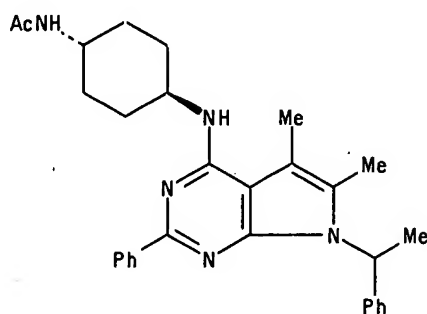
FS STEREOSEARCH

MF C<sub>30</sub>H<sub>35</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:221598

REFERENCE 2:

137:109485

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 28

L2 ANSWER 24 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443760-82-5 REGISTRY

CN Propanamide,

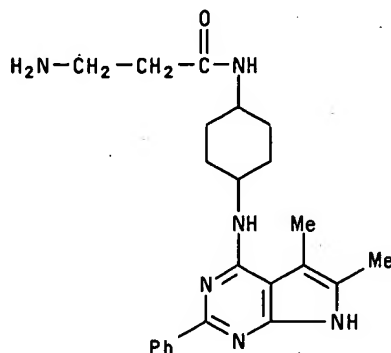
3-amino-N-[4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]cyclohexyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>23</sub>H<sub>30</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109485

\*\*\*\*\*

L2 ANSWER 25 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443760-80-3 REGISTRY

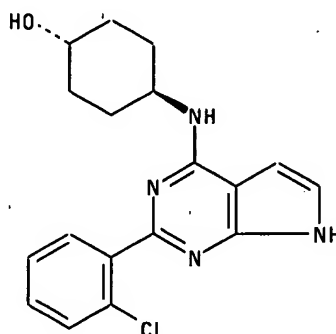
CN Cyclohexanol, 4-[[2-(2-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>18</sub>H<sub>19</sub>ClN<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109485

\*\*\*\*\*

L2 ANSWER 26 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443760-79-0 REGISTRY

CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

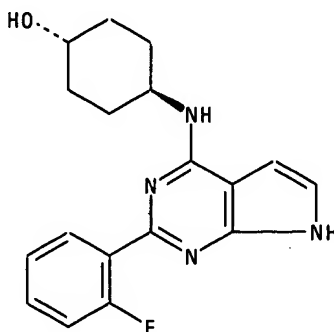
FS STEREOSEARCH

MF C<sub>18</sub>H<sub>19</sub>FN<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109485

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

31

L2 ANSWER 27 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443760-78-9 REGISTRY

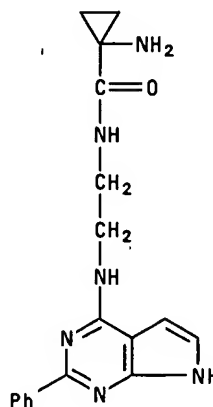
CN Cyclopropanecarboxamide, 1-amino-N-[2-[(2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]ethyl]- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>18</sub>H<sub>20</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109485

\*\*\*\*\*

L2 ANSWER 28 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-78-3 REGISTRY

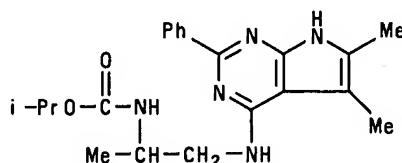
CN Carbamic acid, [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>27</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109288

\*\*\*\*\*

L2 ANSWER 29 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-73-8 REGISTRY

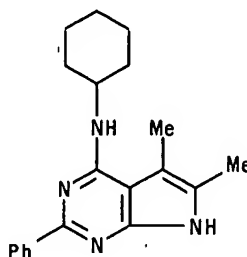
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-cyclohexyl-5,6-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 30 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-72-7 REGISTRY

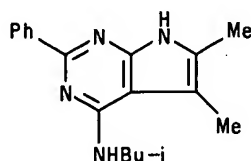
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-*N*-(2-methylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 31 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-71-6 REGISTRY

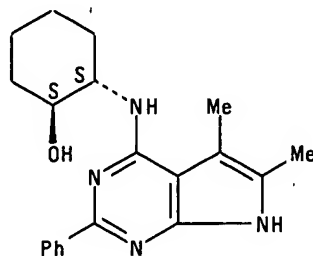
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*S*,2*S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 32 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-70-5 REGISTRY

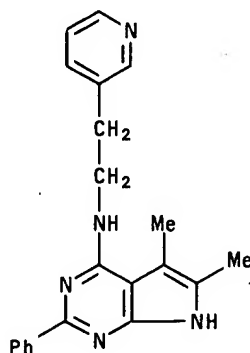
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>21</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 33 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-69-2 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine,

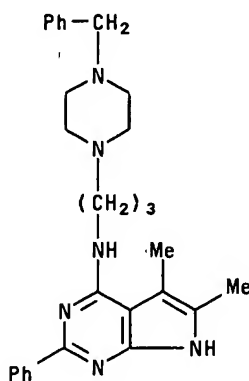
5,6-dimethyl-2-phenyl-*N*-[3-[4-(phenylmethyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>28</sub>H<sub>34</sub>N<sub>6</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 34 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-68-1 REGISTRY

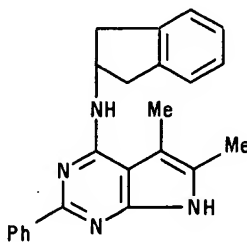
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-(2,3-dihydro-1*H*-inden-2-yl)-5,6-dimethyl-2-phenyl- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>23</sub>H<sub>22</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*



L2 ANSWER 35 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-67-0 REGISTRY

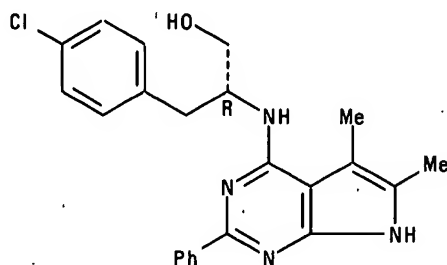
CN Benzenepropanol, 4-chloro- $\beta$ -[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (*βR*)-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>23</sub>H<sub>23</sub>ClN<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 40

L2 ANSWER 36 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-66-9 REGISTRY

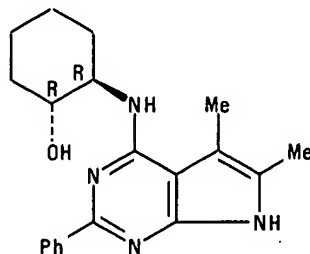
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

41

L2 ANSWER 37 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-65-8 REGISTRY

CN Benzenemethanol,

$\alpha$ -[(1S)-1-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-2-methoxyethyl]-, ( $\alpha R$ )-  
(9CI) (CA INDEX NAME)

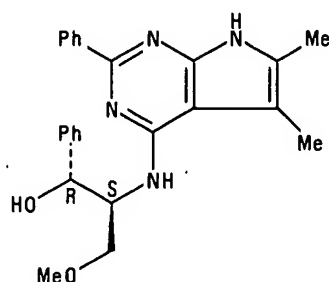
FS STEREOSEARCH

MF C<sub>24</sub>H<sub>26</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 38 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-64-7 REGISTRY

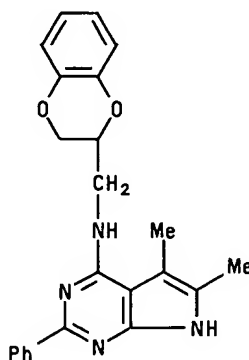
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine,*N*-[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]-5,6-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>23</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

43

L2 ANSWER 39 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-63-6 REGISTRY

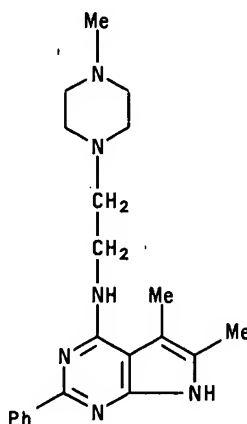
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-*N*-[2-(4-methyl-1-piperazinyl)ethyl]-2-phenyl- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>28</sub>N<sub>6</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 44

L2 ANSWER 40 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-62-5 REGISTRY

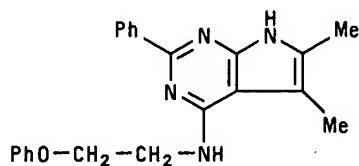
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-*N*-(2-phenoxyethyl)-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 41 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-61-4 REGISTRY

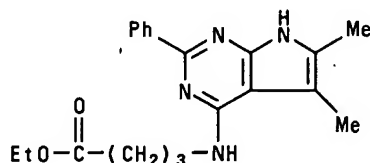
CN Butanoic acid, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, ethyl ester (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

46

L2 ANSWER 42 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-60-3 REGISTRY

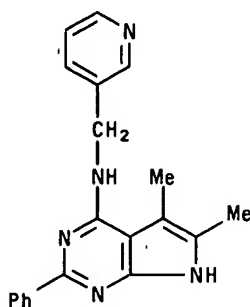
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>19</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

47

L2 ANSWER 43 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-59-0 REGISTRY

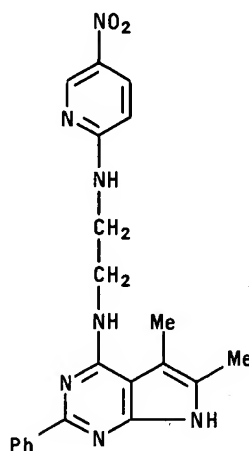
CN 1,2-Ethanediamine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)-*N'*-(5-nitro-2-pyridinyl)-  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>21</sub>N<sub>7</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 44 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-58-9 REGISTRY

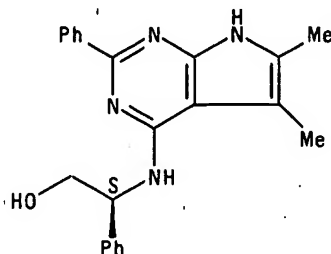
CN Benzeneethanol,  $\beta$ -[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, ( $\beta$ S)- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 45 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-57-8 REGISTRY

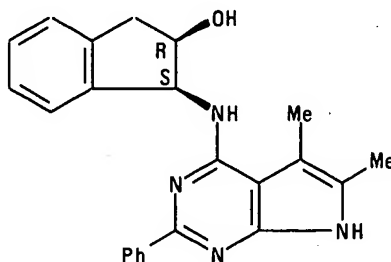
CN 1*H*-Inden-2-ol, 1-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-2,3-dihydro-,  
(1*S*,2*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>23</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 46 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-56-7 REGISTRY

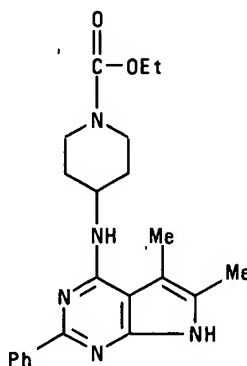
CN 1-Piperidinecarboxylic acid, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>22</sub>H<sub>27</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 47 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-55-6 REGISTRY

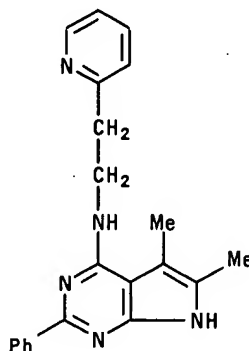
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>21</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

52

L2 ANSWER 48 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-54-5 REGISTRY

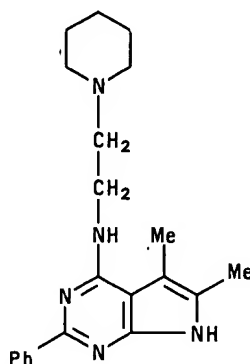
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>27</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 53

L2 ANSWER 49 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-53-4 REGISTRY

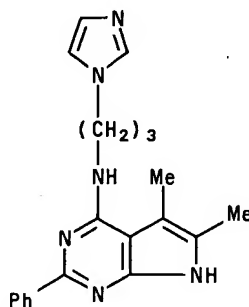
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-[3-(1*H*-imidazol-1-yl)propyl]-5,6-dimethyl-2-phenyl- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>22</sub>N<sub>6</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 50 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-52-3 REGISTRY

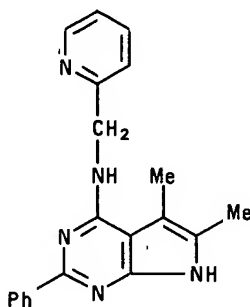
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>19</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 55

L2 ANSWER 51 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-51-2 REGISTRY

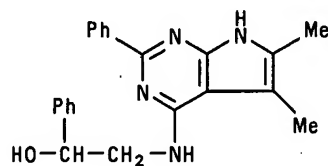
CN Benzenemethanol,  $\alpha$ -[[[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]methyl]- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

56

L2 ANSWER 52 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-50-1 REGISTRY

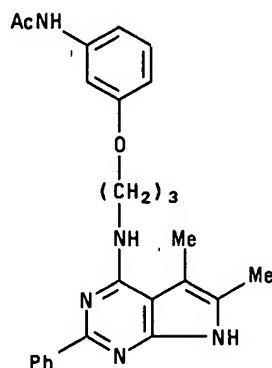
CN Acetamide, *N*-[3-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propoxy]phenyl]-  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>25</sub>H<sub>27</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

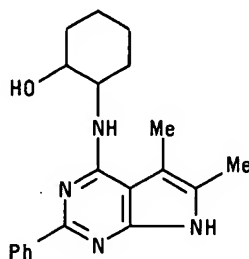
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 53 OF 249 REGISTRY COPYRIGHT 2004 ACS  
 RN 443118-49-8 REGISTRY  
 CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 54 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-48-7 REGISTRY

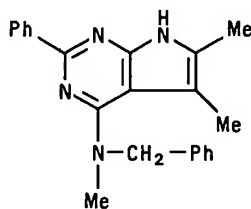
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*,5,6-trimethyl-2-phenyl-*N*-(phenylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 55 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-47-6 REGISTRY

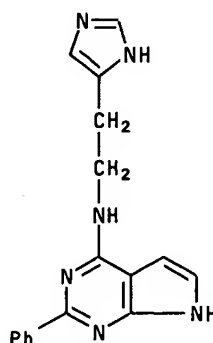
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-[2-(1*H*-imidazol-4-yl)ethyl]-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>17</sub>H<sub>16</sub>N<sub>6</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

REFERENCE 2:

138:321287

REFERENCE 3:

137:109485

REFERENCE 4:

137:109288

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

60

L2 ANSWER 56 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-46-5 REGISTRY

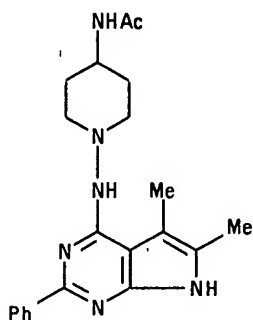
CN Acetamide, *N*-[1-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-4-piperidiny]- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>26</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 57 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-45-4 REGISTRY

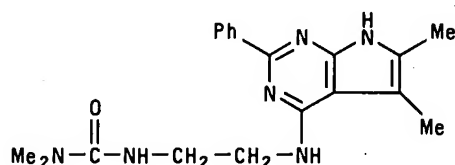
CN Urea, *N'*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-*N,N*-dimethyl-  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>24</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 58 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-44-3 REGISTRY

CN Cyclohexanol,

4-[[5,6-dimethyl-2-phenyl-7-[(1S)-1-phenylethyl]-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, *trans*-  
(9CI) (CA INDEX NAME)

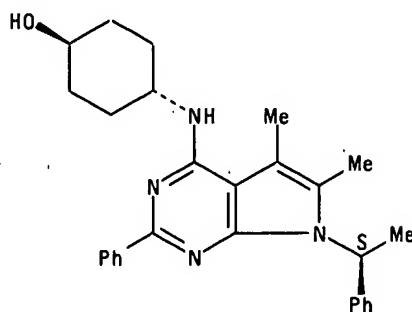
FS STEREOSEARCH

MF C<sub>28</sub>H<sub>32</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

137:109288

\*\*\*\*\*



L2 ANSWER 59 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-43-2 REGISTRY

CN Cyclohexanol,

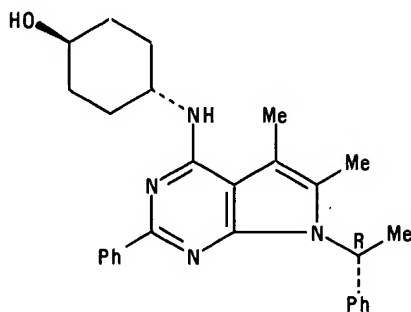
4-[[5,6-dimethyl-2-phenyl-7-[(1*R*)-1-phenylethyl]-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>28</sub>H<sub>32</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109288

\*\*\*\*\*

L2 ANSWER 60 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-42-1 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-*N*-(*trans*-4-methylcyclohexyl)-2-phenyl- (9CI)  
(CA INDEX NAME)

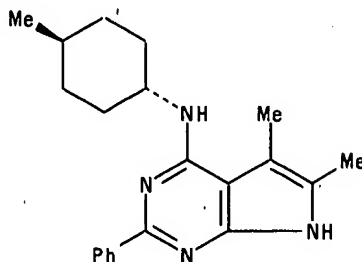
FS STEREOSEARCH

MF C<sub>21</sub>H<sub>26</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

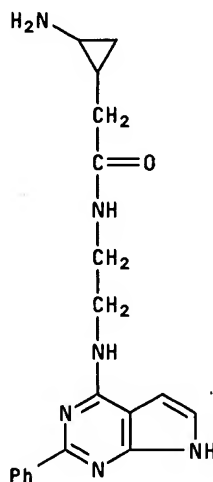
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 61 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 443118-41-0 REGISTRY  
CN Cyclopropaneacetamide, 2-amino-*N*-[2-[(2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]ethyl]- (9CI)  
(CA INDEX NAME)  
FS 3D CONCORD  
MF C<sub>19</sub>H<sub>22</sub>N<sub>6</sub>O  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 62 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-36-3 REGISTRY

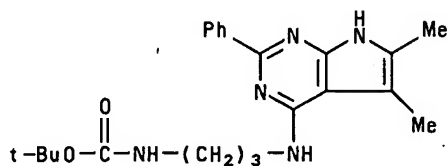
CN Carbamic acid, [3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>22</sub>H<sub>29</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 63 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-26-1 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[*cis*-4-(phenylmethoxy)cyclohexyl]-  
(9CI) (CA INDEX NAME)

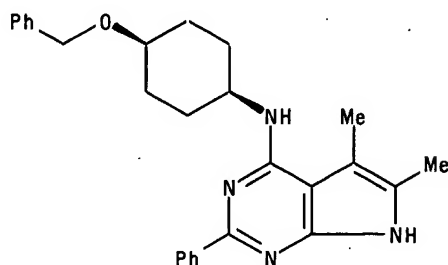
FS STEREOSEARCH

MF C<sub>27</sub>H<sub>30</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 64 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-24-9 REGISTRY

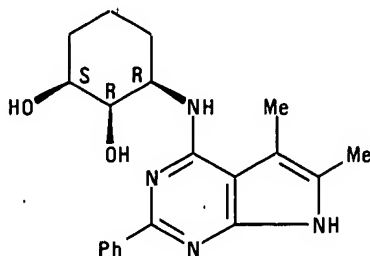
CN 1,2-Cyclohexanediol, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, (1*R*,2*S*,3*S*)-*rel*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
Relative stereochemistry.



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 65 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-23-8 REGISTRY

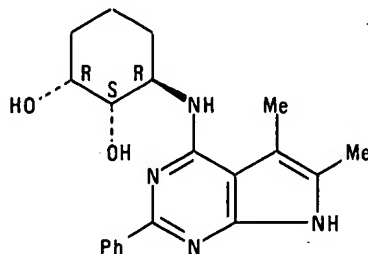
CN 1,2-Cyclohexanediol, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-,  
(1*R*,2*S*,3*R*)-*rel*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 66 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-22-7 REGISTRY

CN Cyclohexanol, 4-[[2-(2-chlorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
(9CI) (CA INDEX NAME)

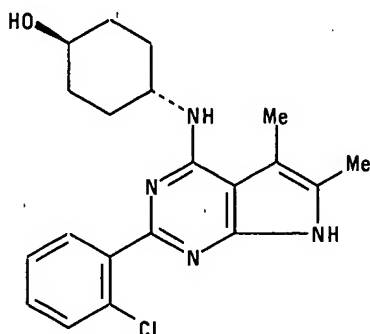
FS STEREOSEARCH

MF C<sub>20</sub>H<sub>23</sub>ClN<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*



L2 ANSWER 67 OF 249 REGISTRY COPYRIGHT 2004 ACS

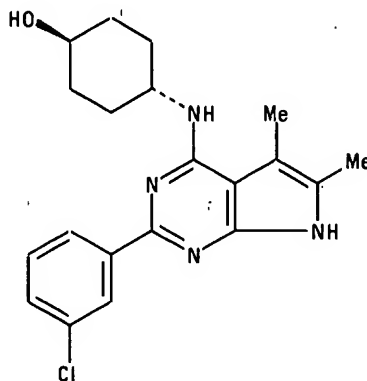
RN 443118-21-6 REGISTRY

CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, *trans*-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>23</sub>ClN<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
Relative stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

\*\*\*\*\*

L2 ANSWER 68 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 412342-10-0 REGISTRY

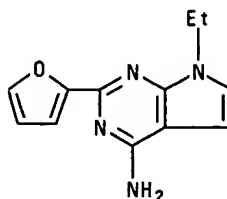
CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 7-ethyl-2-(2-furanyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>12</sub>H<sub>12</sub>N<sub>4</sub>O

SR Reaction Database

LC STN Files: CASREACT



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

73

L2 ANSWER 69 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343969-97-1 REGISTRY

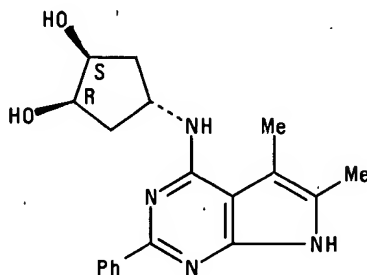
CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, (1 $\alpha$ ,2 $\alpha$ ,4 $\beta$ )-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>19</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

REFERENCE 7:

135:46190

\*\*\*\*\*

L2 ANSWER 70 OF 249 REGISTRY COPYRIGHT 2004 ACS

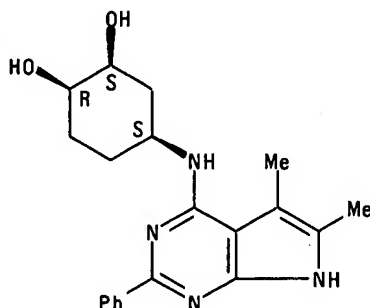
RN 343969-79-9 REGISTRY

CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-,  
(1*R*,2*S*,4*S*)-*rel*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

75

L2 ANSWER 71 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343633-16-9 REGISTRY

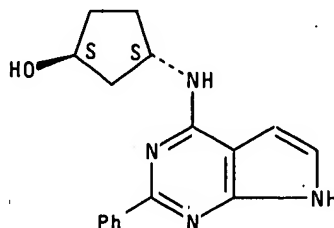
CN Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*S*,3*S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

137:109288

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

76

L2 ANSWER 72 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-97-3 REGISTRY

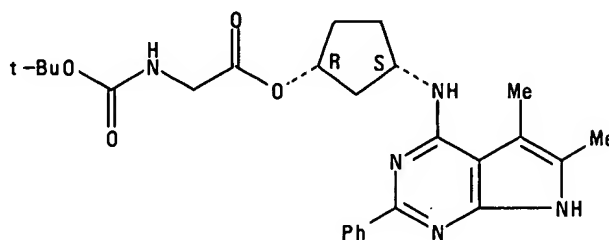
CN Glycine, *N*-[(1,1-dimethylethoxy)carbonyl]-,  
(1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>26</sub>H<sub>33</sub>N<sub>5</sub>O<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:221598

REFERENCE 3:

137:109288

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

77

L2 ANSWER 73 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-96-2 REGISTRY

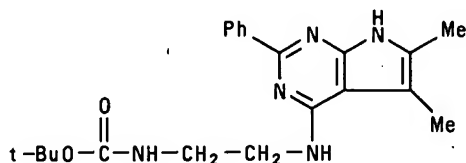
CN Carbamic acid, [2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>27</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

\*\*\*\*\*

L2 ANSWER 74 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-79-1 REGISTRY

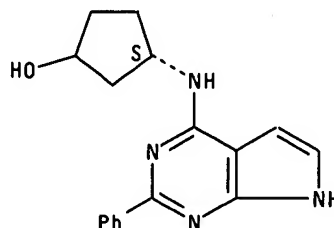
CN Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (3*S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

137:109288

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

\*\*\*\*\*



# STN INTERNATIONAL®

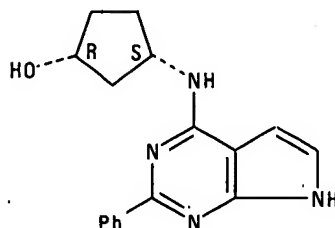
REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

79

L2 ANSWER 75 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 343632-78-0 REGISTRY  
CN Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,3*S*)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)  
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

137:109288

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

80

L2 ANSWER 76 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-77-9 REGISTRY

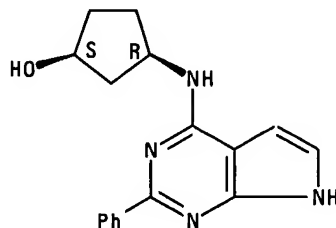
CN Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*S*,3*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

137:109288

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

81

L2 ANSWER 77 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-73-5 REGISTRY

CN Urea,

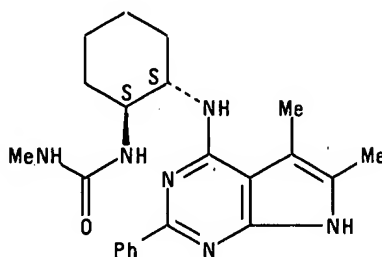
*N*-[(1*S*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-  
(9*CI*) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>22</sub>H<sub>28</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

\*\*\*\*\*

L2 ANSWER 78 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-72-4 REGISTRY

CN Urea,

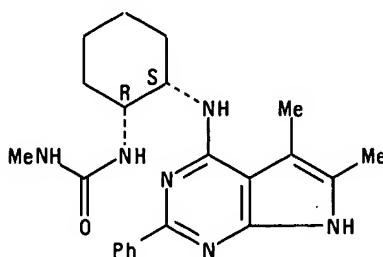
*N*-[(1*R*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>22</sub>H<sub>28</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

83

L2 ANSWER 79 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-71-3 REGISTRY

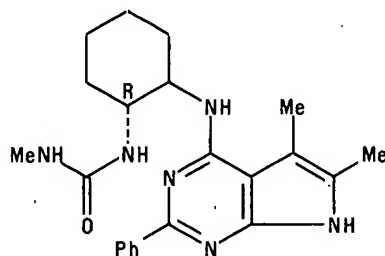
CN Urea, *N*-[(1*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>22</sub>H<sub>28</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

84

L2 ANSWER 80 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-70-2 REGISTRY

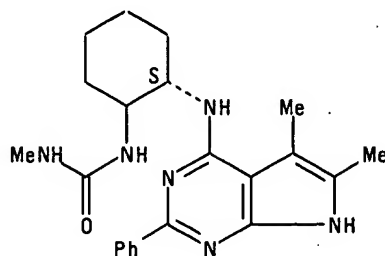
CN Urea, *N*-[(2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>22</sub>H<sub>28</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

85

L2 ANSWER 81 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-69-9 REGISTRY

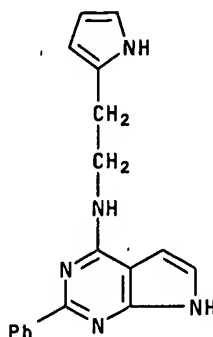
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-phenyl-*N*-[2-(1*H*-pyrrol-2-yl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>18</sub>H<sub>17</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

136:386128

REFERENCE 2:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 86

L2 ANSWER 82 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-50-8 REGISTRY

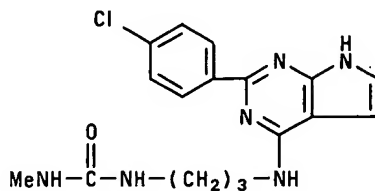
CN Urea, *N*-[3-[[2-(4-chlorophenyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]propyl]-*N'*-methyl- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>17</sub>H<sub>19</sub>ClN<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

135:46190

\*\*\*\*\*



L2 ANSWER 83 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-38-2 REGISTRY

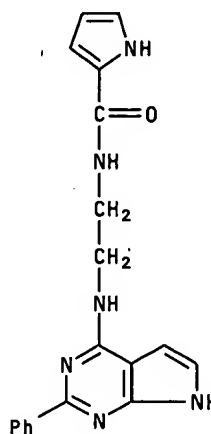
CN 1*H*-Pyrrole-2-carboxamide, *N*-[2-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>18</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

137:109485

REFERENCE 6:

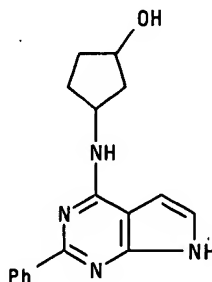
# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 88  
L2 ANSWER 83 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 343632-38-2 REGISTRY  
137:109288

REFERENCE 7:

135:46190

\*\*\*\*\*  
L2 ANSWER 84 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 343632-37-1 REGISTRY  
CN Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)  
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 89

L2 ANSWER 84 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-37-1 REGISTRY

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

135:46190

\*\*\*\*\*

L2 ANSWER 85 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-36-0 REGISTRY

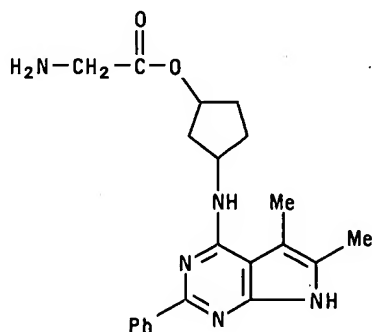
CN Glycine, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]cyclopentyl ester (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>25</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

137:109288

REFERENCE 5:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

91

L2 ANSWER 86 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-35-9 REGISTRY

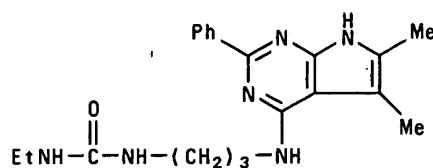
CN Urea, *N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-*N'*-ethyl- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>26</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

135:46190

\*\*\*\*\*

L2 ANSWER 87 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-33-7 REGISTRY

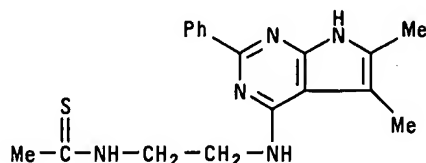
CN Ethanethioamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>18</sub>H<sub>21</sub>N<sub>5</sub>S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

137:109288

REFERENCE 5:

135:46190

\*\*\*\*\*

L2 ANSWER 88 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-32-6 REGISTRY

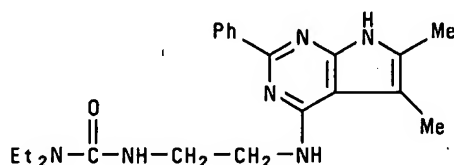
CN Urea, *N'*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]ethyl]-*N,N*-diethyl- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>27</sub>H<sub>28</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

137:109288

REFERENCE 6:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

94

L2 ANSWER 89 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-31-5 REGISTRY

CN Acetamide,

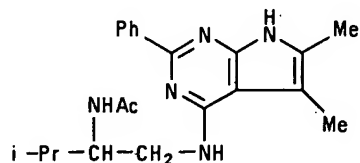
*N*-[1-[[[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]methyl]-2-methylpropyl]- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>27</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

135:46190

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

95

L2 ANSWER 90 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-21-3 REGISTRY

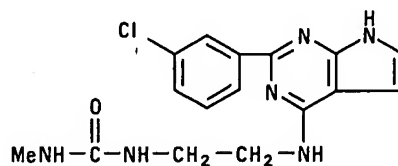
CN Urea, *N*-[2-[[2-(3-chlorophenyl)-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl]amino]ethyl]-*N'*-methyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>16</sub>H<sub>17</sub>ClN<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109485

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

96

L2 ANSWER 91 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-20-2 REGISTRY

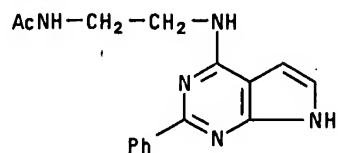
CN Acetamide, *N*-[2-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>16</sub>H<sub>17</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109485

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

97

L2 ANSWER 92 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-19-9 REGISTRY

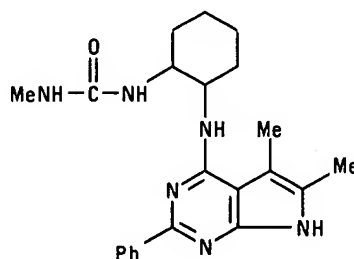
CN Urea, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>22</sub>H<sub>28</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109485

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

\*\*\*\*\*

L2 ANSWER 93 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-17-7 REGISTRY

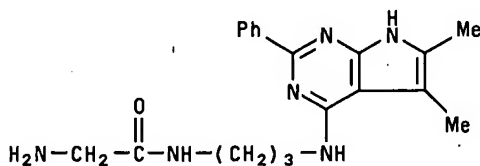
CN Acetamide, 2-amino-*N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>24</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

REFERENCE 7:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

99

L2 ANSWER 94 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-16-6 REGISTRY

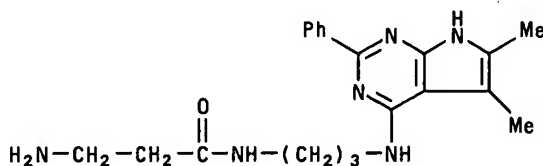
CN Propanamide, 3-amino-*N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]propyl]-  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>26</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109485

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 100

L2 ANSWER 95 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-15-5 REGISTRY

CN Cyclopropanecarboxamide,

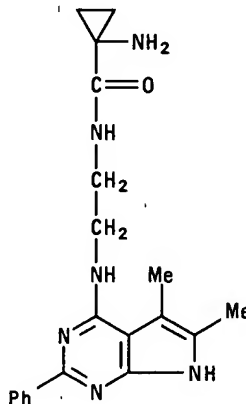
1-amino-*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>24</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109288

REFERENCE 5:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 101

L2 ANSWER 95 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-15-5 REGISTRY

REFERENCE 6:

135:46190

\*\*\*\*\*  
L2 ANSWER 96 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-14-4 REGISTRY

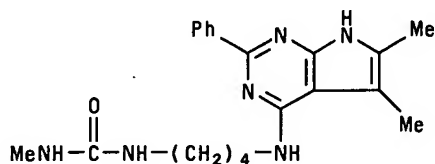
CN Urea, *N*-[4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]butyl]-*N'*-methyl- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>26</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 102  
L2 ANSWER 96 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 343632-14-4 REGISTRY

REFERENCE 7:

135:46190

\*\*\*\*\*  
L2 ANSWER 97 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-13-3 REGISTRY

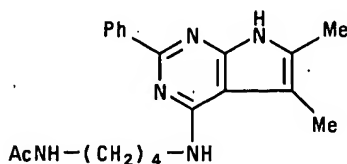
CN Acetamide, *N*-[4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]butyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>25</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 103

L2 ANSWER 97 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-13-3 REGISTRY  
136:386128

REFERENCE 7:

135:46190

\*\*\*\*\*

L2 ANSWER 98 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-12-2 REGISTRY

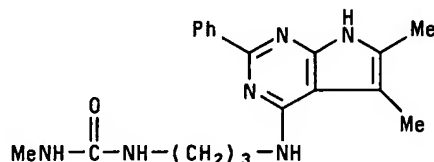
CN Urea, *N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-*N'*-methyl- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>24</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 104

L2 ANSWER 98 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-12-2 REGISTRY

REFERENCE 6:

135:46190

\*\*\*\*\*  
L2 ANSWER 99 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-11-1 REGISTRY

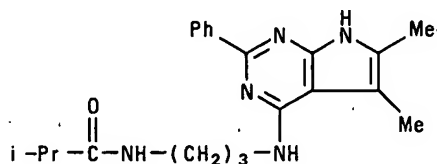
CN Propanamide, *N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-2-methyl-  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>27</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

# STN INTERNATIONAL®

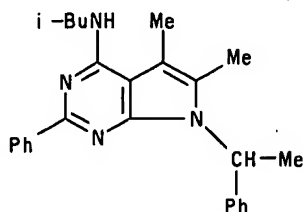
REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 105  
L2 ANSWER 99 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 343632-11-1 REGISTRY

REFERENCE 7:

135:46190

\*\*\*\*\*

L2 ANSWER 100 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 343632-10-0 REGISTRY  
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-*N*-(2-methylpropyl)-2-phenyl-7-(1-phenylethyl)-  
(9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C<sub>26</sub>H<sub>30</sub>N<sub>4</sub>  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)  
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 106

L2 ANSWER 100 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-10-0 REGISTRY

REFERENCE 6:

135:46190

\*\*\*\*\*  
L2 ANSWER 101 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-09-7 REGISTRY

CN Acetamide,

*N*-[2-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]ethyl]- (9CI)

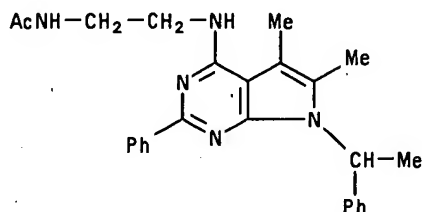
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>26</sub>H<sub>29</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 107

L2 ANSWER 101 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-09-7 REGISTRY

REFERENCE 6:

135:46190

\*\*\*\*\*  
L2 ANSWER 102 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-08-6 REGISTRY

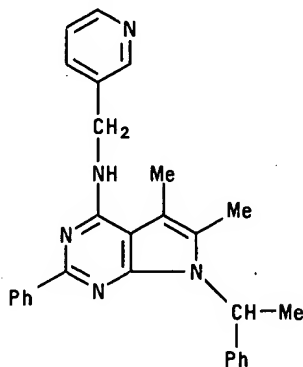
CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-N-(3-pyridinylmethyl)-  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>28</sub>H<sub>27</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 108  
L2 ANSWER 102 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 343632-08-6 REGISTRY

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

\*\*\*\*\*  
L2 ANSWER 103 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-07-5 REGISTRY

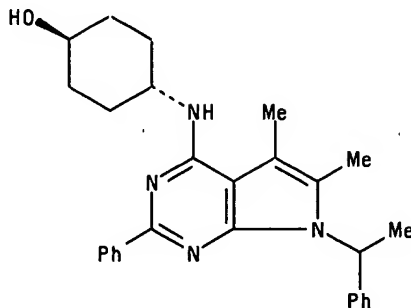
CN Cyclohexanol, 4-[[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>28</sub>H<sub>32</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 109

L2 ANSWER 103 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-07-5 REGISTRY

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 110

L2 ANSWER 104 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-06-4 REGISTRY

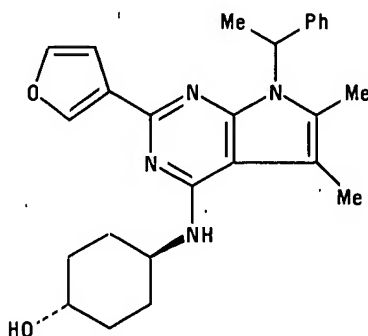
CN Cyclohexanol, 4-[[2-(3-furanyl)-5,6-dimethyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>26</sub>H<sub>30</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

137:109485

REFERENCE 4:

137:109288

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 111

L2 ANSWER 105 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-05-3 REGISTRY

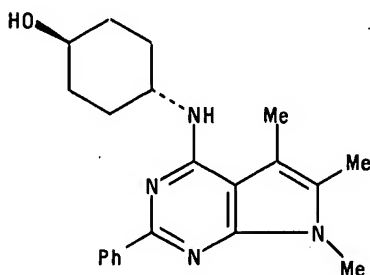
CN Cyclohexanol, 4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d']pyrimidin-4-yl)amino]-, *trans*- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>21</sub>H<sub>26</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

\*\*\*\*\*

L2 ANSWER 106 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-04-2 REGISTRY

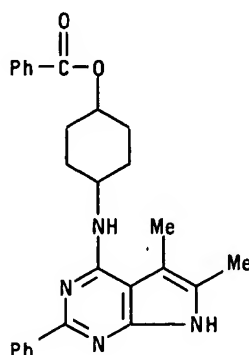
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, benzoate (ester)  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>27</sub>H<sub>28</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109288

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

\*\*\*\*\*

L2 ANSWER 107 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-03-1 REGISTRY

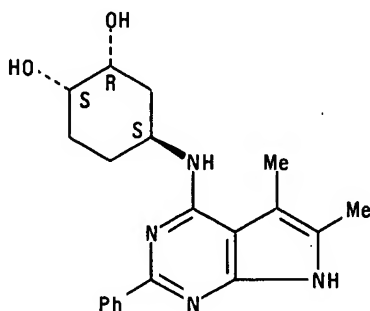
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*S*,4*R*)-*rel*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 114

L2 ANSWER 108 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343631-99-2 REGISTRY

CN Acetamide,

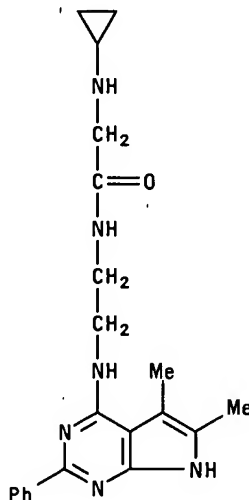
2-(cyclopropylamino)-*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>26</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

\*\*\*\*\*

L2 ANSWER 109 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343631-97-0 REGISTRY

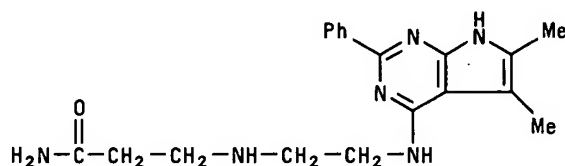
CN Propanamide, 3-[[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]amino]- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>24</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 116

L2 ANSWER 110 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343631-96-9 REGISTRY

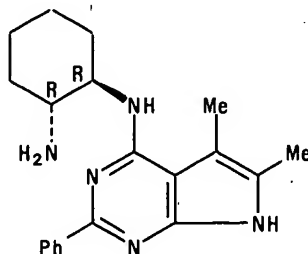
CN 1,2-Cyclohexanediamine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)-, (1*R*,2*R*)- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>25</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 117

L2 ANSWER 111 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343631-95-8 REGISTRY

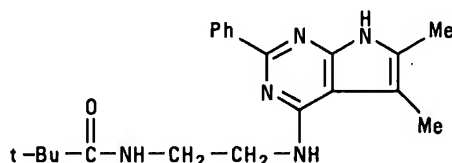
CN Propanamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2,2-dimethyl-  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>27</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

\*\*\*\*\*

L2 ANSWER 112 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 341964-52-1 REGISTRY

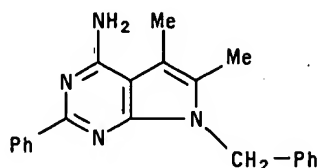
CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>20</sub>N<sub>4</sub>

SR Chemical Library

LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

\*\*\*\*\*



L2 ANSWER 113 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-50-0 REGISTRY

CN 1-Butanol,

2-[[2-(4-chlorophenyl)-5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-7*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl]amino]-  
(9*CI*) (CA INDEX NAME)

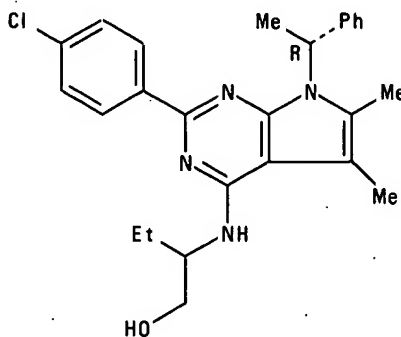
FS STEREOSEARCH

MF C<sub>26</sub>H<sub>29</sub>ClN<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 120

L2 ANSWER 114 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-49-7 REGISTRY

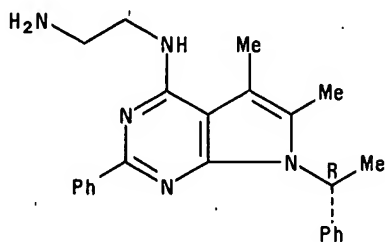
CN 1,2-Ethanediamine, *N*-[5,6-dimethyl-2-phenyl-7-[(1*R*)-1-phenylethyl]-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>24</sub>H<sub>27</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT  
Absolute stereochemistry.



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 121

L2 ANSWER 115 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-48-6 REGISTRY

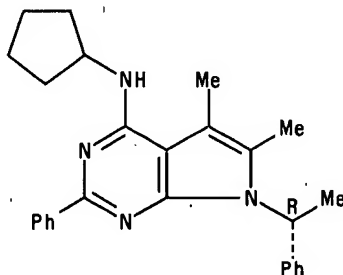
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, *N*-cyclopentyl-5,6-dimethyl-2-phenyl-7-[(1*R*)-1-phenylethyl]-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>27</sub>H<sub>30</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

L2 ANSWER 116 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-47-5 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*,7-bis[(1*R*)-1-phenylethyl]- (9CI) (CA INDEX NAME)

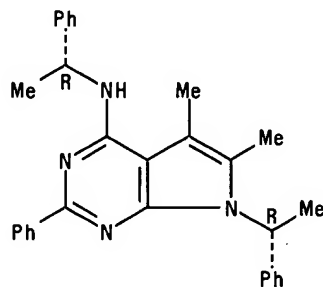
FS STEREOSEARCH

MF C<sub>30</sub>H<sub>30</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 123

L2 ANSWER 117 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-41-9 REGISTRY

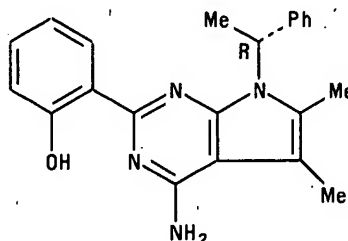
CN Phenol, 2-[4-amino-5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-7*H*-pyrrolo[2,3-*d'*]pyrimidin-2-yl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, CASREACT  
Absolute stereochemistry.



\*\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 124

L2 ANSWER 118 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-39-5 REGISTRY

CN 2-Propenoic acid,

3-[[[5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-(4-pyridinyl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, methyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

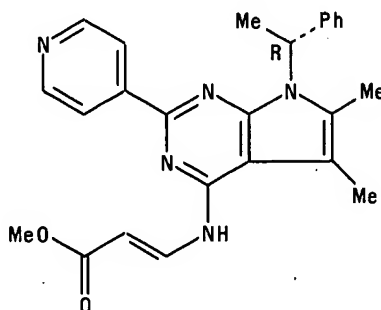
MF C<sub>25</sub>H<sub>25</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

Double bond geometry unknown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

L2 ANSWER 119 OF 249 REGISTRY COPYRIGHT 2004 ACS

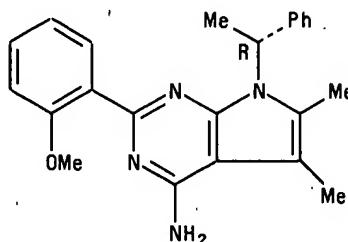
RN 319481-26-0 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(2-methoxyphenyl)-5,6-dimethyl-7-[(1*R*)-1-phenylethyl]- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>23</sub>H<sub>24</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, CASREACT  
Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

L2 ANSWER 120 OF 249 REGISTRY COPYRIGHT 2004 ACS

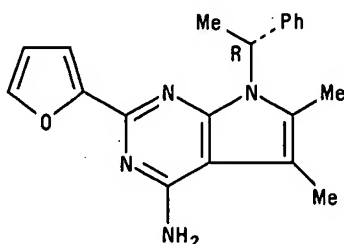
RN 319481-25-9 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(2-furanyl)-5,6-dimethyl-7-[(1*R*)-1-phenylethyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>20</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, CASREACT  
Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*



L2 ANSWER 121 OF 249 REGISTRY COPYRIGHT 2004 ACS

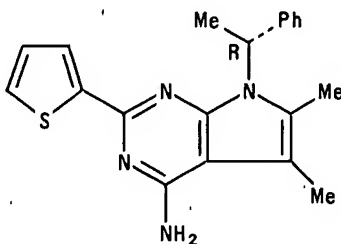
RN 319481-24-8 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-(2-thienyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>20</sub>N<sub>4</sub>S

SR CA

LC STN Files: CA, CAPLUS, CASREACT  
Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

L2 ANSWER 122 OF 249 REGISTRY COPYRIGHT 2004 ACS

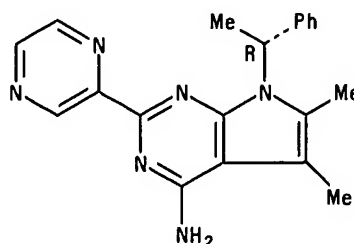
RN 319481-23-7 REGISTRY

CN 7H-Pyrrolo[2,3-d']pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-pyrazinyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>20</sub>N<sub>6</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT  
Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

L2 ANSWER 123 OF 249 REGISTRY COPYRIGHT 2004 ACS

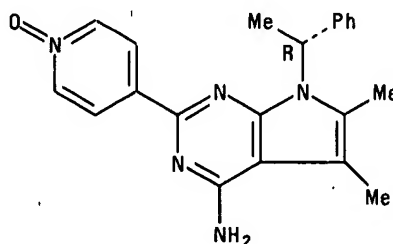
RN 319481-22-6 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-2-(1-oxido-4-pyridinyl)-7-[(1*R*)-1-phenylethyl]- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>21</sub>H<sub>21</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, CASREACT  
Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

L2 ANSWER 124 OF 249 REGISTRY COPYRIGHT 2004 ACS

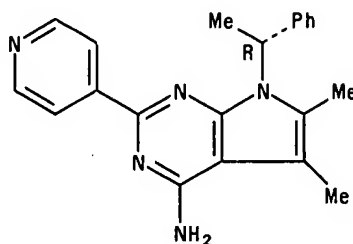
RN 319481-21-5 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>21</sub>H<sub>21</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT  
Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 131

L2 ANSWER 125 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-20-4 REGISTRY

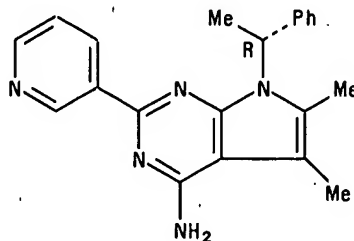
CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-(3-pyridinyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>21</sub>H<sub>21</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT  
Absolute stereochemistry.



\*\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

L2 ANSWER 126 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-19-1 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)

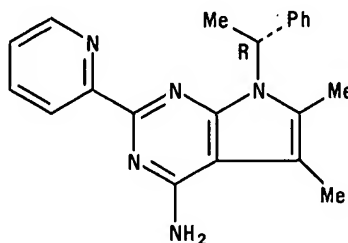
FS STEREOSEARCH

MF C<sub>21</sub>H<sub>21</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 133

L2 ANSWER 127 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251947-24-7 REGISTRY

CN Methanesulfonamide,

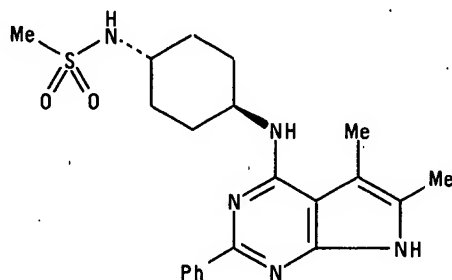
*N*-[*trans*-4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>21</sub>H<sub>27</sub>N<sub>5</sub>O<sub>2</sub>S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

138:221598

REFERENCE 6:

137:109485

REFERENCE 7:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 134

L2 ANSWER 127 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251947-24-7 REGISTRY

137:109288

REFERENCE 8:

136:386128

REFERENCE 9:

135:46190

REFERENCE 10:

132:22973

\*\*\*\*\*



L2 ANSWER 128 OF 249 REGISTRY COPYRIGHT 2004 ACS

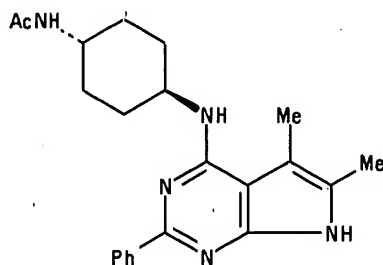
RN 251947-22-5 REGISTRY

CN Acetamide, *N*-[*trans*-4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>22</sub>H<sub>27</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

138:221598

REFERENCE 6:

137:109485

REFERENCE 7:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 136  
L2 ANSWER 128 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 251947-22-5 REGISTRY

REFERENCE 8:

136:386128

REFERENCE 9:

135:46190

REFERENCE 10:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 137

L2 ANSWER 129 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-59-5 REGISTRY

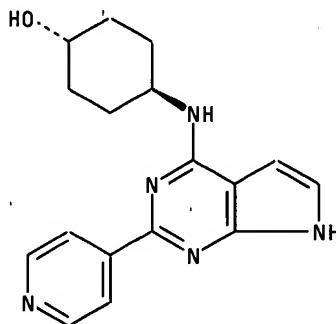
CN Cyclohexanol, 4-[[2-(4-pyridinyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>17</sub>H<sub>19</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 138

L2 ANSWER 129 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-59-5 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 130 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-58-4 REGISTRY

CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

OTHER NAMES:

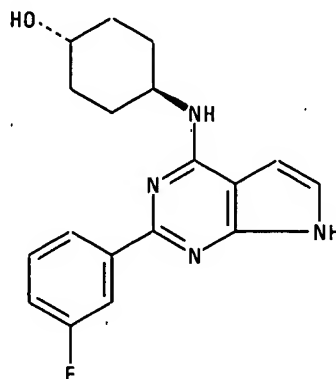
CN 4-[(*trans*-4-Hydroxycyclohexyl)amino]-2-(3-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C<sub>18</sub>H<sub>19</sub>FN<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 140

L2 ANSWER 130 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-58-4 REGISTRY

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 131 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-57-3 REGISTRY

CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(*trans*-4-Hydroxycyclohexyl)amino]-2-(3-chlorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

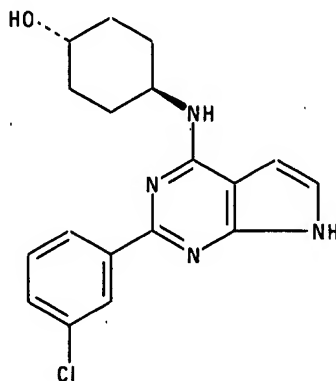
FS STEREOSEARCH

MF C<sub>18</sub>H<sub>19</sub>ClN<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 142

L2 ANSWER 131 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-57-3 REGISTRY

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 143

L2 ANSWER 132 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-56-2 REGISTRY

CN Urea, *N*-[1-[[[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]methyl]propyl]-*N'*-methyl-  
(9CI) (CA INDEX NAME)

OTHER NAMES:

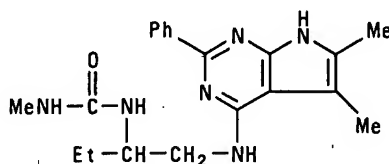
CN 4-[[2-(*N'*-Methylureido)butyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>20</sub>H<sub>26</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

REFERENCE 7:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 144

L2 ANSWER 133 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-55-1 REGISTRY

CN Acetamide, *N*-[1-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]methyl]propyl]- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

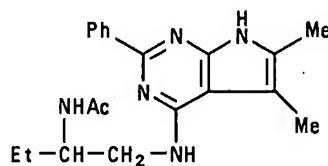
CN 4-[(2-Acetamidobutyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidiné

FS 3D CONCORD

MF C<sub>20</sub>H<sub>25</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

REFERENCE 7:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 145

L2 ANSWER 134 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-54-0 REGISTRY

CN Urea, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-*N'*-methyl-  
(9CI) (CA INDEX NAME)

OTHER NAMES:

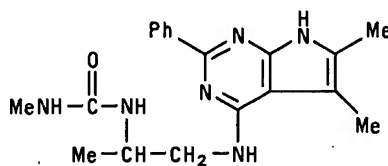
CN 4-[[2-(*N'*-Methylureido)propyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>19</sub>H<sub>24</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

REFERENCE 7:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 146

L2 ANSWER 135 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-52-8 REGISTRY

CN Glycine, (1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>21</sub>H<sub>25</sub>N<sub>5</sub>O<sub>2</sub>.C<sub>2</sub>HF<sub>3</sub>O<sub>2</sub>

SR CA

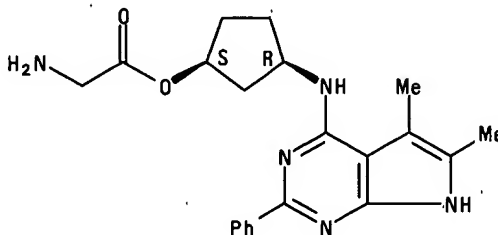
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

CM 1

CRN 251946-51-7

CMF C<sub>21</sub>H<sub>25</sub>N<sub>5</sub>O<sub>2</sub>

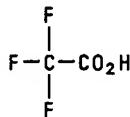
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C<sub>2</sub>HF<sub>3</sub>O<sub>2</sub>



6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

137:109485

REFERENCE 3:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 147

L2 ANSWER 135 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-52-8 REGISTRY  
137:109288

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

REFERENCE 6:

132:22973

\*\*\*\*\*  
L2 ANSWER 136 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-51-7 REGISTRY

CN Glycine, (1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*- (9CI) (CA INDEX NAME)

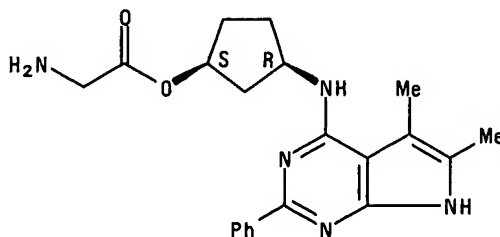
FS STEREOSEARCH

MF C<sub>21</sub>H<sub>25</sub>N<sub>5</sub>O<sub>2</sub>

CI COM

SR CA

Relative stereochemistry.



\*\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*\*

\*\*\*\*\*

L2 ANSWER 137 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-50-6 REGISTRY

CN Butanoic acid,

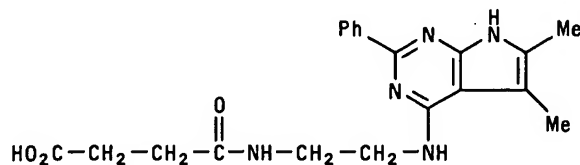
4-[[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>23</sub>N<sub>5</sub>O<sub>3</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

REFERENCE 7:

135:46190

REFERENCE 8:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 149

L2 ANSWER 137 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-50-6 REGISTRY  
132:22973

\*\*\*\*\*  
L2 ANSWER 138 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-49-3 REGISTRY

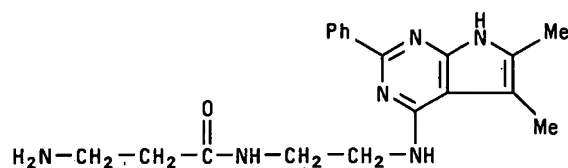
CN Propanamide, 3-amino-*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]ethyl]-  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>24</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:  
140:146159

REFERENCE 2:  
139:133575

REFERENCE 3:  
138:221598

REFERENCE 4:  
137:109485

REFERENCE 5:  
137:109288

REFERENCE 6:  
136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 150

L2 ANSWER 138 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-49-3 REGISTRY

REFERENCE 7:

135:46190

REFERENCE 8:

132:22973

\*\*\*\*\*

L2 ANSWER 139 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-48-2 REGISTRY

CN Ethanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, acetate (ester) (9CI)  
(CA INDEX NAME)

OTHER NAMES:

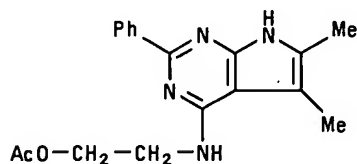
CN 4-[(2-Acetyloxyethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>18</sub>H<sub>20</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 151

L2 ANSWER 139 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-48-2 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 152

L2 ANSWER 140 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-47-1 REGISTRY

CN Acetamide, *N*-[(1*R*,2*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN (*R,R*)-4-[(2-Acetylamino)cyclohexyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

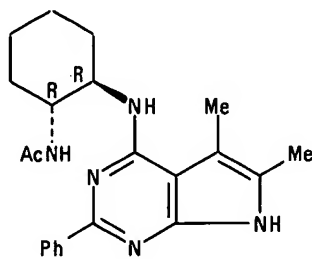
FS STEREOSEARCH

MF C<sub>22</sub>H<sub>27</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 153

L2 ANSWER 140 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-47-1 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 154

L2 ANSWER 141 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-46-0 REGISTRY

CN Acetamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

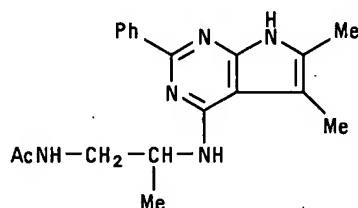
CN 4-[(1-Methyl-2-acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 155

L2 ANSWER 141 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-46-0 REGISTRY

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 142 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-45-9 REGISTRY

CN Acetamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1,1-dimethylethyl]-  
(9CI) (CA INDEX NAME)

OTHER NAMES:

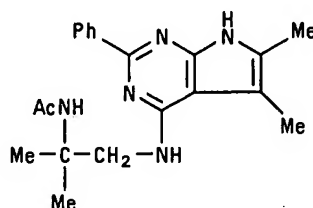
CN 4-[(2-Methyl-2-acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>20</sub>H<sub>25</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 157

L2 ANSWER 142 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-45-9 REGISTRY

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 158

L2 ANSWER 143 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-44-8 REGISTRY

CN Acetamide, *N*-[(1*S*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-  
(9CI) (CA INDEX NAME)

OTHER NAMES:

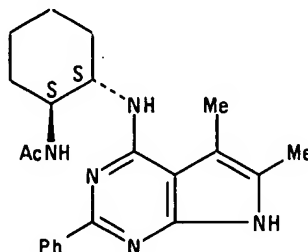
CN (*S,S*)-4-[(2-Acetylaminocyclohexyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C<sub>22</sub>H<sub>27</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 159

L2 ANSWER 143 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-44-8 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 160

L2 ANSWER 144 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-43-7 REGISTRY

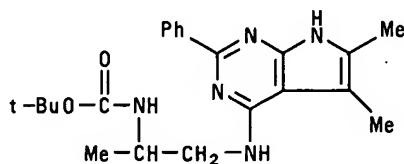
CN Carbamic acid, [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>22</sub>H<sub>29</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

137:109485

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

REFERENCE 6:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 161

L2 ANSWER 145 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-42-6 REGISTRY

CN Carbamic acid, [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

OTHER NAMES:

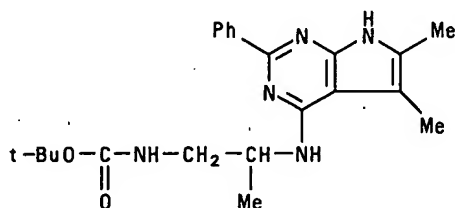
CN 4-[[1-Methyl-2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS 3D CONCORD

MF C<sub>22</sub>H<sub>29</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 162

L2 ANSWER 145 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-42-6 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 146 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-41-5 REGISTRY

CN Acetamide, *N*-[(2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]propyl]- (9CI)  
(CA INDEX NAME)

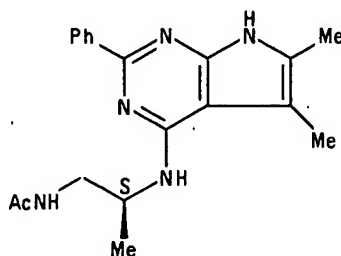
## OTHER NAMES:

CN (S)-4-[(1-Methyl-2-acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS STEREOSEARCH

MF C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 164

L2 ANSWER 146 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-41-5 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 165

L2 ANSWER 147 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-40-4 REGISTRY

CN Acetamide, *N*-[(1*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-  
(9CI) (CA INDEX NAME)

OTHER NAMES:

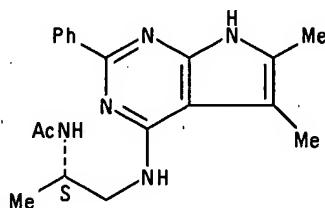
CN (S)-4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 166

L2 ANSWER 147 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-40-4 REGISTRY

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 167

L2 ANSWER 148 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-39-1 REGISTRY

CN Acetamide, *N*-[(2*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

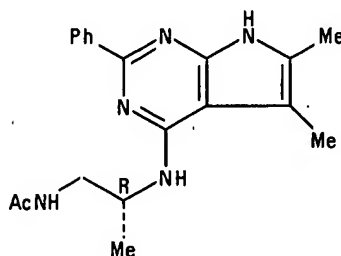
CN (*R*)-4-[(1-Methyl-2-acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 168

L2 ANSWER 148 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-39-1 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 169

L2 ANSWER 149 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-38-0 REGISTRY

CN Acetamide, *N*-[(1*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-  
(9CI) (CA INDEX NAME)

OTHER NAMES:

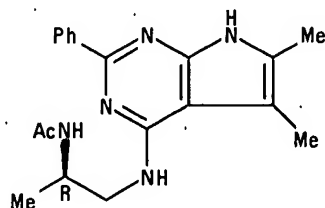
CN (*R*)-4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 170  
L2 ANSWER 149 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 251946-38-0 REGISTRY  
136:386128

REFERENCE 8:  
135:46190

REFERENCE 9:  
132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 171

L2 ANSWER 150 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-37-9 REGISTRY

CN Acetamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

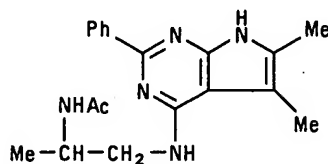
CN 4-[(2-Acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 172

L2 ANSWER 150 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-37-9 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 151 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-36-8 REGISTRY

CN Urea, [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

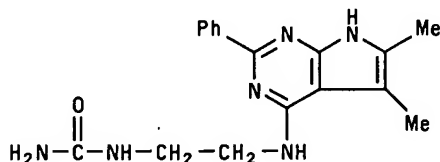
CN 4-[(2-Ureidoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>17</sub>H<sub>20</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 173

L2 ANSWER 151 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-36-8 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 152 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-35-7 REGISTRY

CN Propanamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2-oxo- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

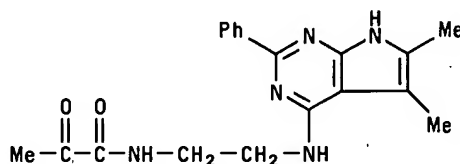
CN 4-[(2-Pyruvylamidoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>19</sub>H<sub>21</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 175

L2 ANSWER 152 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-35-7 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*  
L2 ANSWER 153 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-34-6 REGISTRY

CN Urea, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-*N'*-ethyl- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

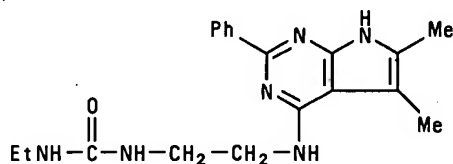
CN 4-[[2-(*N'*-Ethylureido)ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>19</sub>H<sub>24</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 176

L2 ANSWER 153 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-34-6 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 177

L2 ANSWER 154 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-33-5 REGISTRY

CN Urea, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-*N'*-methyl- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

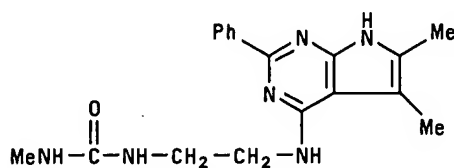
CN 4-[[2-(*N'*-Methylureido)ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>18</sub>H<sub>22</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 178

L2 ANSWER 154 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-33-5 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 155 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-32-4 REGISTRY

CN Propanamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

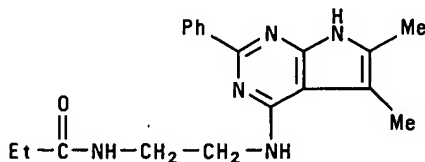
CN 4-[(2-Propionylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 179

L2 ANSWER 155 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-32-4 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 180

L2 ANSWER 156 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-31-3 REGISTRY

CN 1,2-Ethanediamine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

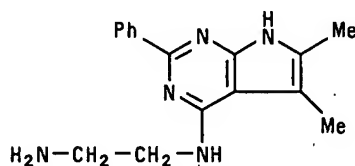
CN 4-[(2-Aminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>16</sub>H<sub>19</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 181

L2 ANSWER 156 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-31-3 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*  
L2 ANSWER 157 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-30-2 REGISTRY

CN Methanesulfonamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

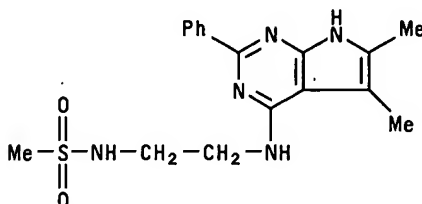
CN 4-[[2-(Methylsulfonylamino)ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>17</sub>H<sub>21</sub>N<sub>5</sub>O<sub>2</sub>S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 182  
L2 ANSWER 157 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 251946-30-2 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*



L2 ANSWER 158 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-29-9 REGISTRY

CN Propanamide, *N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

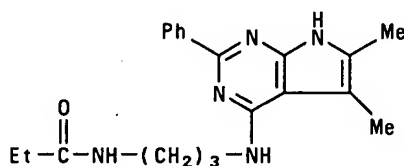
CN 4-[(3-Propionylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>20</sub>H<sub>25</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 184

L2 ANSWER 158 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-29-9 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*  
L2 ANSWER 159 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-28-8 REGISTRY

CN Propanamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2-methyl-  
(9CI) (CA INDEX NAME)

OTHER NAMES:

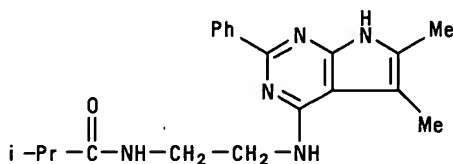
CN 4-[(2-Isobutrylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>20</sub>H<sub>25</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 185

L2 ANSWER 159 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-28-8 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 160 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-27-7 REGISTRY

CN Cyclopropanecarboxamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-  
(9CI) (CA INDEX NAME)

## OTHER NAMES:

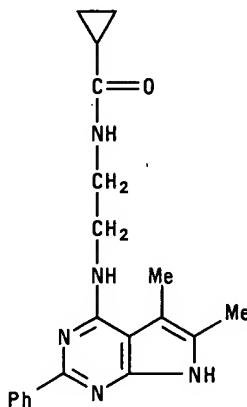
CN 4-[[2-[(Cyclopropanecarbonyl)amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>20</sub>H<sub>23</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 187  
L2 ANSWER 160 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 251946-27-7 REGISTRY

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 188

L2 ANSWER 161 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-26-6 REGISTRY

CN Propanamide, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-*N*-methyl- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

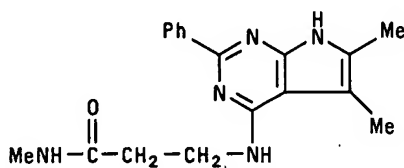
CN 4-[[3-(Methylamino)-3-oxopropyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS 3D CONCORD

MF C<sub>18</sub>H<sub>21</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 189

L2 ANSWER 161 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-26-6 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 162 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-25-5 REGISTRY

CN 1,3-Propanediamine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

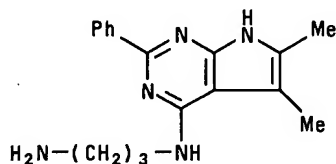
CN 4-[(3-Aminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>17</sub>H<sub>21</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 190

L2 ANSWER 162 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-25-5 REGISTRY

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

REFERENCE 7:

135:46190

REFERENCE 8:

132:22973

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 191

L2 ANSWER 163 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-24-4 REGISTRY

CN  $\beta$ -Alanine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

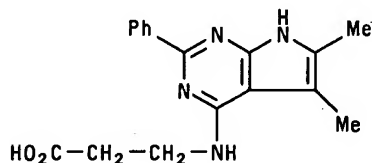
CN 4-[(3-Hydroxy-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS 3D CONCORD

MF C<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 192

L2 ANSWER 163 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-24-4 REGISTRY

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 164 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-23-3 REGISTRY

CN Acetamide, *N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

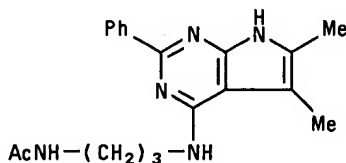
CN 4-[(3-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 193

L2 ANSWER 164 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-23-3 REGISTRY

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 194

L2 ANSWER 165 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-22-2 REGISTRY

CN Formamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

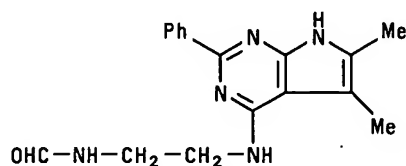
CN 4-[(2-Formylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>17</sub>H<sub>19</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 195

L2 ANSWER 165 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-22-2 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*  
L2 ANSWER 166 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-21-1 REGISTRY

CN Propanamide, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-*N,N*-dimethyl- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

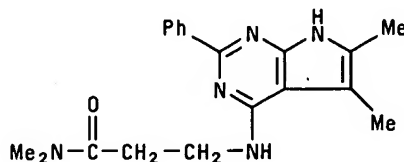
CN 4-[[3-(Dimethylamino)-3-oxopropyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 196

L2 ANSWER 166 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-21-1 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 197

L2 ANSWER 167 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-20-0 REGISTRY

CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, *cis*- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*cis*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

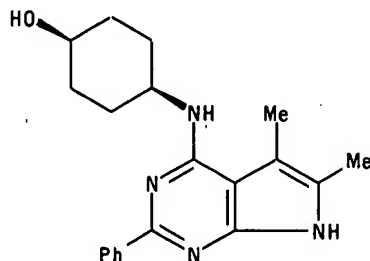
FS STEREOSEARCH

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 198

L2 ANSWER 167 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-20-0 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 199

L2 ANSWER 168 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-19-7 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-3-cyclohexen-1-yl-5,6-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

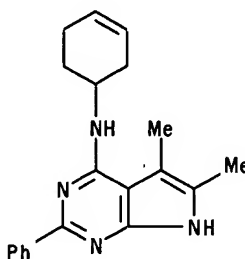
CN 4-[(3-Cyclohexenyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>20</sub>H<sub>22</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 200

L2 ANSWER 168 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-19-7 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 169 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-18-6 REGISTRY

CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, benzoate (ester), *cis*- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*cis*-Benzoyloxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

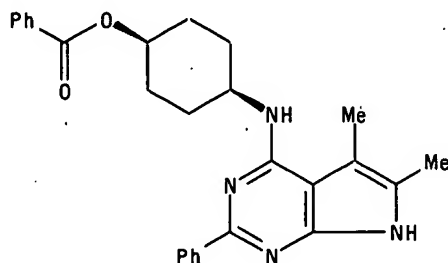
FS STEREOSEARCH

MF C<sub>27</sub>H<sub>28</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 202

L2 ANSWER 169 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-18-6 REGISTRY

REFERENCE 7:

135:46190

REFERENCE 8:

132:22973

\*\*\*\*\*

L2 ANSWER 170 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-17-5 REGISTRY

CN 1-Butanol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

OTHER NAMES:

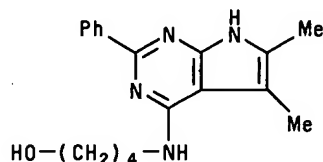
CN 4-[(4-Hydroxybutyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 203

L2 ANSWER 170 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-17-5 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 171 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-16-4 REGISTRY

CN 1-Propanol, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

OTHER NAMES:

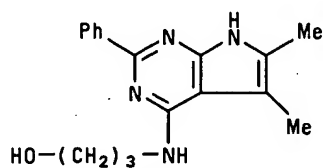
CN 4-[(3-Hydroxypropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>17</sub>H<sub>20</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 205

L2 ANSWER 171 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-16-4 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 172 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-15-3 REGISTRY

CN Ethanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

OTHER NAMES:

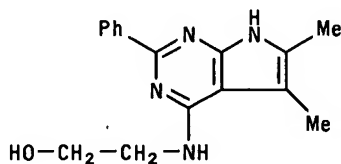
CN 4-[(2-Hydroxyethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>16</sub>H<sub>18</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 206

L2 ANSWER 172 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-15-3 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 207

L2 ANSWER 173 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-14-2 REGISTRY

CN  $\beta$ -Alanine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)-, 1,1-dimethylethyl ester (9CI)  
(CA INDEX NAME)

OTHER NAMES:

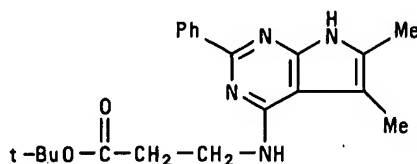
CN 4-[(3-*tert*-Butyloxy-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS 3D CONCORD

MF C<sub>21</sub>H<sub>26</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 208

L2 ANSWER 173 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-14-2 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 174 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-13-1 REGISTRY

CN Acetamide, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-*N*-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

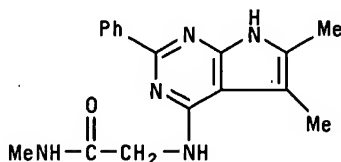
CN 4-[[2-(Methylamino)-2-oxoethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>17</sub>H<sub>19</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 209

L2 ANSWER 174 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-13-1 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 210

L2 ANSWER 175 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-12-0 REGISTRY

CN Acetamide, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

OTHER NAMES:

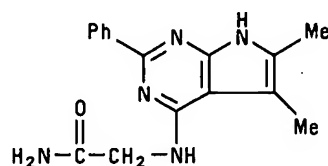
CN 4-[(2-Amino-2-oxoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>16</sub>H<sub>17</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 211

L2 ANSWER 175 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-12-0 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 176 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-11-9 REGISTRY

CN Propanamide, *N*-(cyclopropylmethyl)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-(9CI) (CA INDEX NAME)

OTHER NAMES:

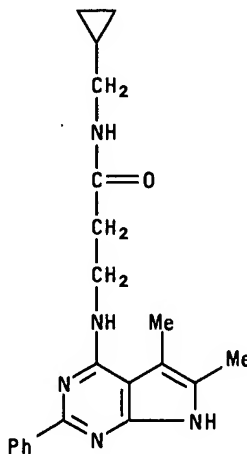
CN 4-[[3-(Cyclopropylmethylamino)-3-oxopropyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>21</sub>H<sub>25</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 212

L2 ANSWER 176 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-11-9 REGISTRY

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

138:221598

REFERENCE 6:

137:109485

REFERENCE 7:

137:109288

REFERENCE 8:

136:386128

REFERENCE 9:

135:46190

REFERENCE 10:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 213

L2 ANSWER 177 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-10-8 REGISTRY

CN Propanamide, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

OTHER NAMES:

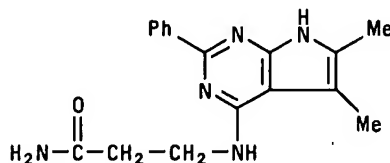
CN 4-[(3-Amino-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>17</sub>H<sub>19</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 214

L2 ANSWER 177 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-10-8 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*  
L2 ANSWER 178 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-09-5 REGISTRY

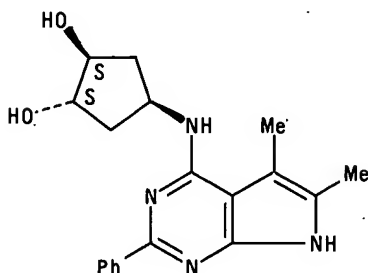
CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, stereoisomer (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>19</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 215  
L2 ANSWER 178 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 251946-09-5 REGISTRY

REFERENCE 5:

132:22973

\*\*\*\*\*

L2 ANSWER 179 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-08-4 REGISTRY

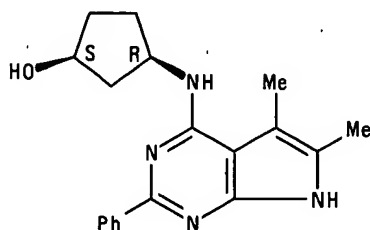
CN Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,3*S*)-*rel*- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>19</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 216  
L2 ANSWER 179 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 251946-08-4 REGISTRY

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 217

L2 ANSWER 180 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-07-3 REGISTRY

CN Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,3*R*)-*rel*- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

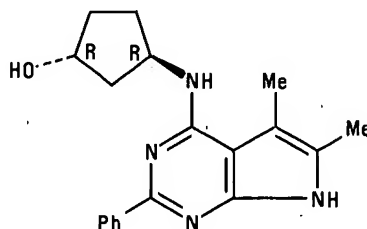
CN 4-[(3-*trans*-Hydroxycyclopentyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C<sub>19</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 218

L2 ANSWER 180 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-07-3 REGISTRY

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 181 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-06-2 REGISTRY

CN Cyclopentanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(2-*trans*-Hydroxycyclopentyl)amino]-5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidine

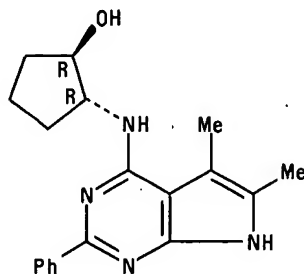
FS STEREOSEARCH

MF C<sub>19</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 220

L2 ANSWER 181 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-06-2 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 182 OF 249 REGISTRY COPYRIGHT 2004 ACS

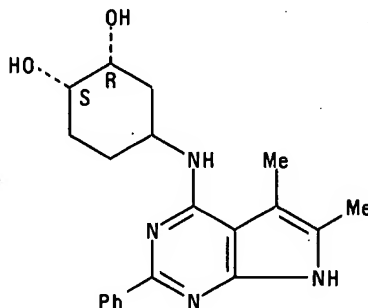
RN 251946-05-1 REGISTRY

CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*S*)-*rel*-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

REFERENCE 5:

132:22973

\*\*\*\*\*

L2 ANSWER 183 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-04-0 REGISTRY

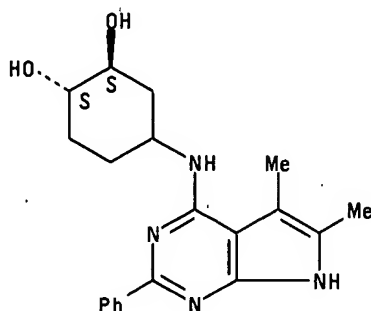
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

REFERENCE 5:

132:22973

\*\*\*\*\*



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 223

L2 ANSWER 184 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-03-9 REGISTRY

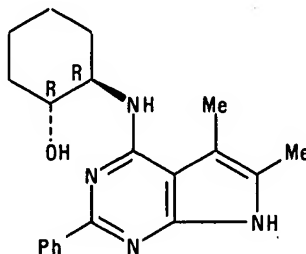
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109288

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

REFERENCE 7:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 224

L2 ANSWER 185 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-01-7 REGISTRY

CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

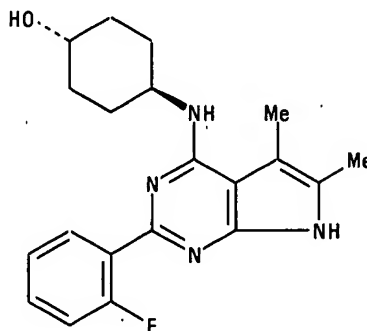
FS STEREOSEARCH

MF C<sub>20</sub>H<sub>23</sub>FN<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 225

L2 ANSWER 185 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-01-7 REGISTRY

136:386128

REFERENCE 7:

135:46190

REFERENCE 8:

132:22973

\*\*\*\*\*

L2 ANSWER 186 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-00-6 REGISTRY

CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

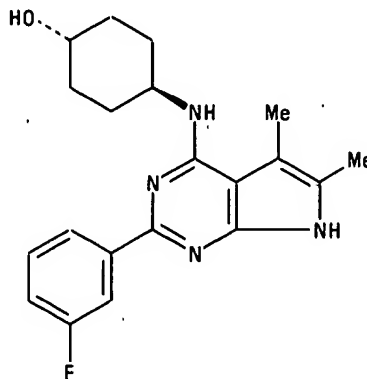
FS STEREOSEARCH

MF C<sub>20</sub>H<sub>23</sub>FN<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 227

L2 ANSWER 186 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-00-6 REGISTRY

REFERENCE 6:

136:386128

REFERENCE 7:

135:46190

REFERENCE 8:

132:22973

\*\*\*\*\*

L2 ANSWER 187 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-99-0 REGISTRY

CN Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(4-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

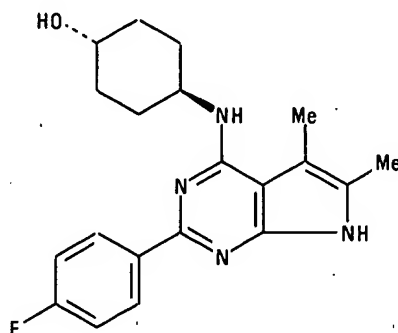
FS STEREOSEARCH

MF C<sub>20</sub>H<sub>23</sub>FN<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 229  
L2 ANSWER 187 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 251945-99-0 REGISTRY  
136:386128

REFERENCE 7:  
135:46190

REFERENCE 8:  
132:22973

\*\*\*\*\*

L2 ANSWER 188 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-98-9 REGISTRY

CN Cyclohexanol, 4-[[5,6-dimethyl-2-(3-thienyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-thienyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

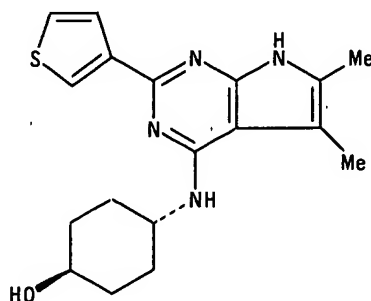
FS STEREOSEARCH

MF C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>OS

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 231

L2 ANSWER 188 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-98-9 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 189 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-97-8 REGISTRY

CN Cyclohexanol, 4-[[5,6-dimethyl-2-(2-thienyl)-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl]amino]-, *trans*- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-thienyl)-7*H*-pyrrolo[2,3-*d'*]pyrimidine

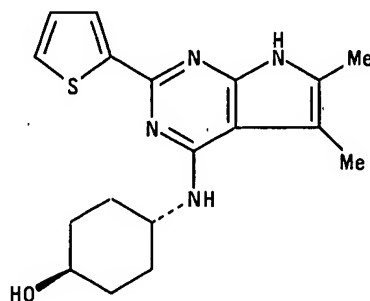
FS STEREOSEARCH

MF C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>OS

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 233  
L2 ANSWER 189 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 251945-97-8 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 190 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-96-7 REGISTRY

CN Cyclohexanol, 4-[(2-cyclopentyl-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-cyclopentyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

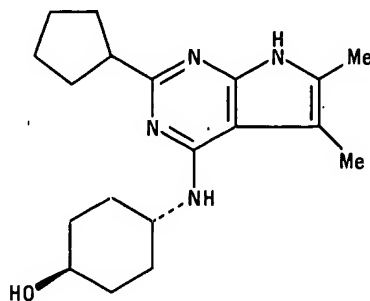
FS STEREOSEARCH

MF C<sub>19</sub>H<sub>28</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 235  
L2 ANSWER 190 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 251945-96-7 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 236

L2 ANSWER 191 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-95-6 REGISTRY

CN Cyclohexanol, 4-[[2-(3-furanyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

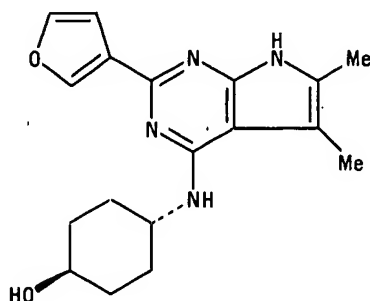
CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-furyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 237  
L2 ANSWER 191 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 251945-95-6 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 238

L2 ANSWER 192 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-94-5 REGISTRY

CN Cyclohexanol, 4-[[2-(2-furanyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-furyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

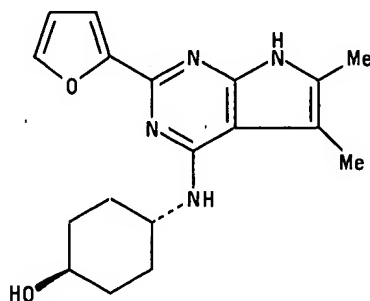
FS STEREOSEARCH

MF C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 239

L2 ANSWER 192 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-94-5 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

L2 ANSWER 193 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-93-4 REGISTRY

CN Cyclohexanol, 4-[[5,6-dimethyl-2-(3-pyridinyl)-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl]amino]-, *trans*- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-pyridyl)-7*H*-pyrrolo[2,3-*d'*]pyrimidine

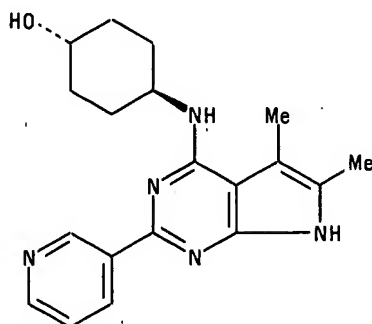
FS STEREOSEARCH

MF C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 241

L2 ANSWER 193 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-93-4 REGISTRY

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 242

L2 ANSWER 194 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-92-3 REGISTRY

CN Cyclohexanol, 4-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*- (9CI) (CA INDEX NAME)

OTHER NAMES:

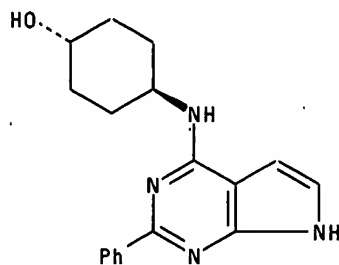
CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C<sub>18</sub>H<sub>20</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 243

L2 ANSWER 194 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-92-3 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 244

L2 ANSWER 195 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-91-2 REGISTRY

CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, *trans*- (9CI) (CA INDEX NAME)

OTHER NAMES:

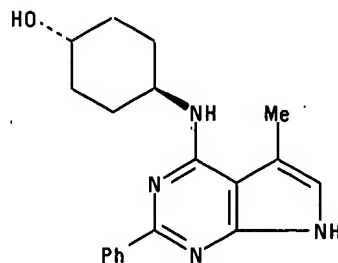
CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5-methyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS STEREOSEARCH

MF C<sub>19</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 245

L2 ANSWER 195 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-91-2 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 246

L2 ANSWER 196 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-90-1 REGISTRY

CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*- (9CI) (CA INDEX NAME)

OTHER NAMES:

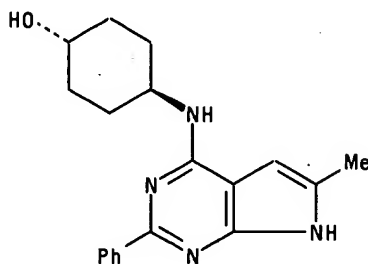
CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-6-methyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C<sub>19</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL  
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 247

L2 ANSWER 196 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-90-1 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

\*\*\*\*\*  
L2 ANSWER 197 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-48-1 REGISTRY

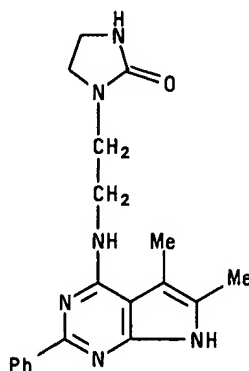
CN 2-Imidazolidinone, 1-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]ethyl]- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>19</sub>H<sub>22</sub>N<sub>6</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

REFERENCE 2:

131:281026  
\*\*\*\*\*

L2 ANSWER 198 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-47-0 REGISTRY

CN 1*H*-Inden-1-ol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-2,3-dihydro-, (1*R*,2*R*)-*rel*- (9CI) (CA INDEX NAME)

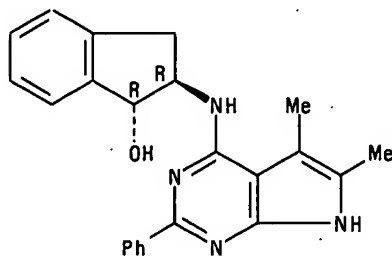
FS STEREOSEARCH

MF C<sub>23</sub>H<sub>22</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS

Relative stereochemistry.



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:281026

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 249

L2 ANSWER 199 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-46-9 REGISTRY

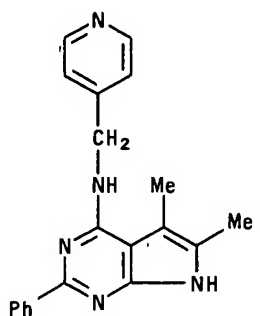
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>20</sub>H<sub>19</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

REFERENCE 2:

131:281026

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 250

L2 ANSWER 200 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-45-8 REGISTRY

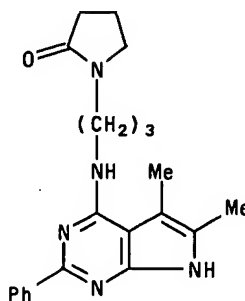
CN 2-Pyrrolidinone, 1-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]- (9CI)  
(CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>25</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

REFERENCE 2:

131:281026

\*\*\*\*\*

L2 ANSWER 201 OF 249 REGISTRY COPYRIGHT 2004 ACS

**RN 246855-44-7 REGISTRY**

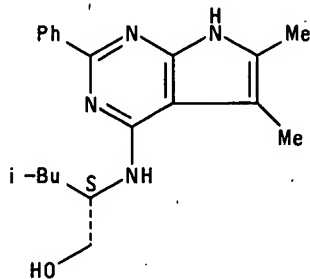
**CN** 1-Pentanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-4-methyl-, (2*S*)- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

**MF** **C<sub>20</sub>H<sub>26</sub>N<sub>4</sub>O**

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
Absolute stereochemistry.



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

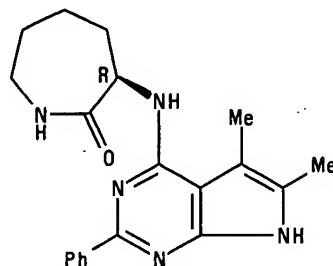
**137:109288**

REFERENCE 2:

**131:281026**

[illegible]

L2 ANSWER 202 OF 249 REGISTRY COPYRIGHT 2004 ACS  
 RN 246855-43-6 REGISTRY  
 CN 2*H*-Azepin-2-one, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]hexahydro-, (3*R*)-  
 (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C<sub>20</sub>H<sub>23</sub>N<sub>5</sub>O  
 SR CA  
 LC STN Files: CA, CAPLUS  
 Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:281026

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 253

L2 ANSWER 203 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-42-5 REGISTRY

CN Acetamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

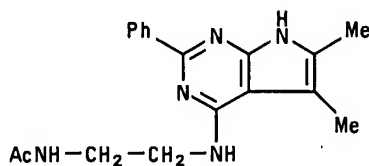
CN 4-[(2-Acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C<sub>18</sub>H<sub>21</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 254

L2 ANSWER 203 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-42-5 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

REFERENCE 10:

131:281026

\*\*\*\*\*



L2 ANSWER 204 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-41-4 REGISTRY

CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*- (9CI) (CA INDEX NAME)

## OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

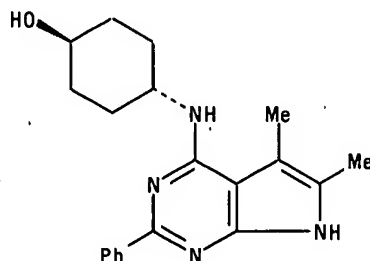
FS STEREOSEARCH

MF C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*.

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1:

140:146159

## REFERENCE 2:

139:133575

## REFERENCE 3:

138:321287

## REFERENCE 4:

138:221598

## REFERENCE 5:

137:109485

## REFERENCE 6:

137:109288

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 256

L2 ANSWER 204 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-41-4 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

REFERENCE 10:

131:281026

L2 ANSWER 205 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-81-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-7-[(methoxyacetyl)amino]-8-oxo-, monosodium salt,  
(6*R*,7*R*)- (9CI) (CA INDEX NAME)

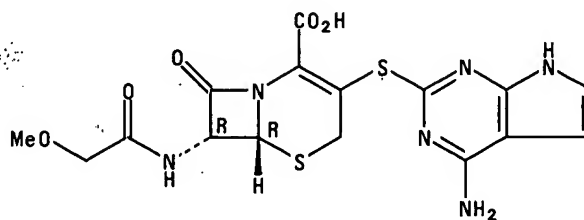
FS STEREOSEARCH

MF C<sub>16</sub>H<sub>16</sub>N<sub>6</sub>O<sub>5</sub>S<sub>2</sub>.Na

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



• Na

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

L2 ANSWER 206 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-78-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
7-(acetylamino)-3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-8-oxo-, monosodium salt, (6*R*,7*R*)-  
(9CI) (CA INDEX NAME)

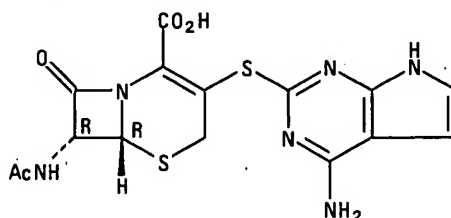
FS STEREOSEARCH

MF C<sub>15</sub>H<sub>14</sub>N<sub>6</sub>O<sub>4</sub>S<sub>2</sub>.Na

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



• Na

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

\*\*\*\*\*

L2 ANSWER 207 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-54-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-7-[(methoxyacetyl)amino]-8-oxo-, diphenylmethyl  
ester, (6*R*,7*R*)- (9CI) (CA INDEX NAME)

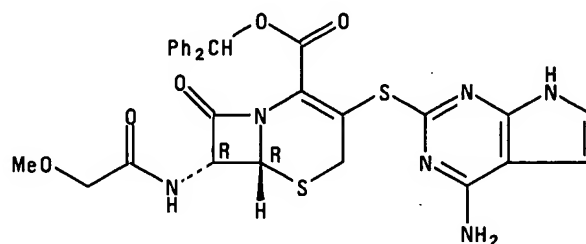
FS STEREOSEARCH

MF C<sub>29</sub>H<sub>26</sub>N<sub>6</sub>O<sub>5</sub>S<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 259

L2 ANSWER 208 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-50-0 REGISTRY

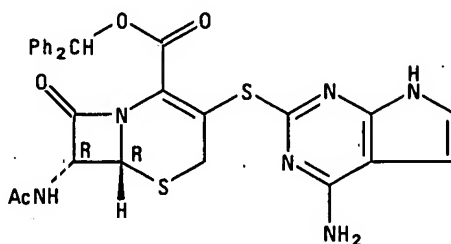
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
7-(acetylamino)-3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-8-oxo-, diphenylmethyl ester,  
(6*R*,7*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>28</sub>H<sub>24</sub>N<sub>6</sub>O<sub>4</sub>S<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

\*\*\*\*\*

L2 ANSWER 209 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-28-2 REGISTRY

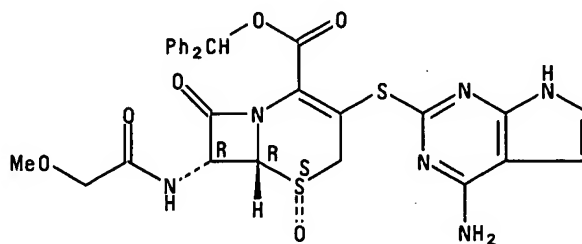
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-7-[(methoxyacetyl)amino]-8-oxo-, diphenylmethyl  
ester, 5-oxide, (5*S*,6*R*,7*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>29</sub>H<sub>26</sub>N<sub>6</sub>O<sub>6</sub>S<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

\*\*\*\*\*

L2 ANSWER 210 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-25-9 REGISTRY

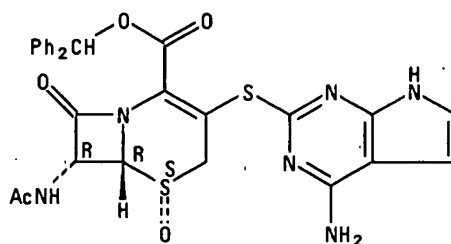
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
7-(acetylamino)-3-[(4-amino-1*H*-pyrrolo[2,3-*d'*]pyrimidin-2-yl)thio]-8-oxo-, diphenylmethyl ester,  
5-oxide, (5*S*,6*R*,7*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>28</sub>H<sub>24</sub>N<sub>6</sub>O<sub>5</sub>S<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

\*\*\*\*\*

L2 ANSWER 211 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245487-76-7 REGISTRY

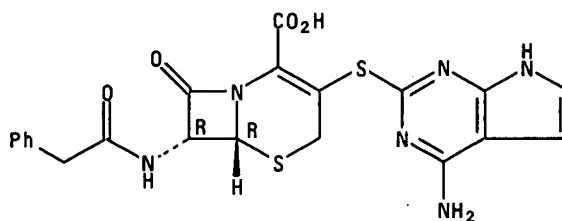
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-8-oxo-7-[(phenylacetyl)amino]-, monosodium salt,  
(6*R*,7*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>21</sub>H<sub>18</sub>N<sub>6</sub>O<sub>4</sub>S<sub>2</sub>.Na

SR CA

LC STN Files: CA, CAPLUS  
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

\*\*\*\*\*



L2 ANSWER 212 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245487-14-3 REGISTRY

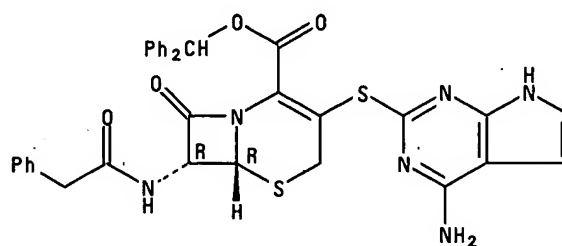
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-8-oxo-7-[(phenylacetyl)amino]-, diphenylmethyl  
ester, (6*R*,7*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>34</sub>H<sub>28</sub>N<sub>6</sub>O<sub>4</sub>S<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

\*\*\*\*\*

L2 ANSWER 213 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245486-48-0 REGISTRY

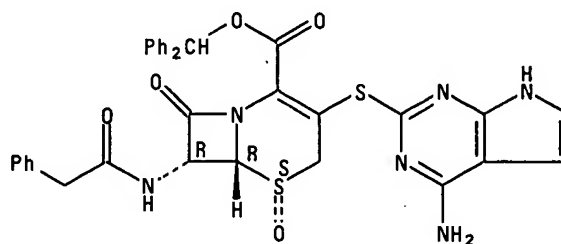
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-8-oxo-7-[(phenylacetyl)amino]-, diphenylmethyl  
ester, 5-oxide, (5*S*,6*R*,7*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>34</sub>H<sub>28</sub>N<sub>6</sub>O<sub>5</sub>S<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

\*\*\*\*\*

L2 ANSWER 214 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 206197-05-9 REGISTRY

CN 7H-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-methyl-2-phenylethyl]-2-phenyl- (9CI)  
(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7H-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-7-(1-methyl-2-phenylethyl)-2-phenyl-, (*R*)-

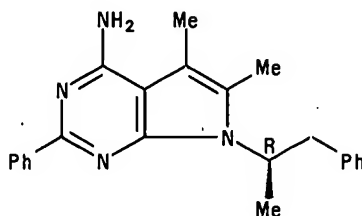
FS STEREOSEARCH

MF C<sub>23</sub>H<sub>24</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

128:299556

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 266

L2 ANSWER 215 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 181862-16-8 REGISTRY

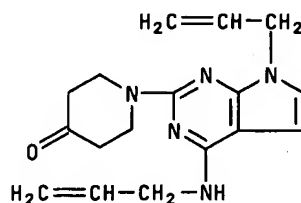
CN 4-Piperidinone, 1-[7-(2-propenyl)-4-(2-propenylamino)-7H-pyrrolo[2,3-d']pyrimidin-2-yl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>17</sub>H<sub>21</sub>N<sub>5</sub>O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:237579

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 267

L2 ANSWER 216 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 181862-15-7 REGISTRY

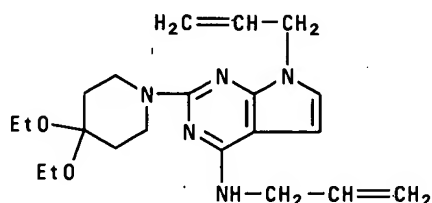
CN 7H-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(4,4-diethoxy-1-piperidiny)-*N*,7-di-2-propenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>31</sub>N<sub>5</sub>O<sub>2</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:237579

\*\*\*\*\*

L2 ANSWER 217 OF 249 REGISTRY COPYRIGHT 2004 ACS

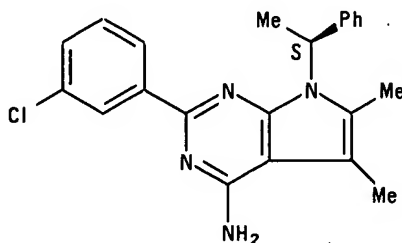
RN 177570-35-3 REGISTRY

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(3-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (S)- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>22</sub>H<sub>21</sub>ClN<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS  
Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

\*\*\*\*\*

L2 ANSWER 218 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 177570-34-2 REGISTRY

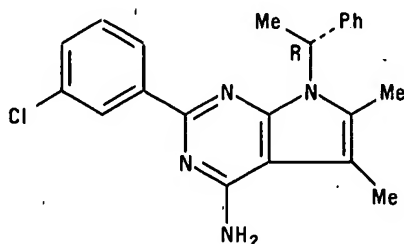
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(3-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (*R*)- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>22</sub>H<sub>21</sub>ClN<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

\*\*\*\*\*

L2 ANSWER 219 OF 249 REGISTRY COPYRIGHT 2004 ACS

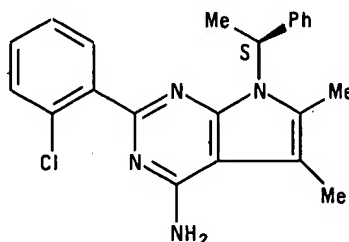
RN 177570-33-1 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(2-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (*S*)- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>22</sub>H<sub>21</sub>ClN<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS  
Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

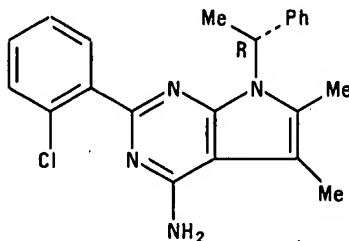
REFERENCE 1:

125:25634

\*\*\*\*\*



L2 ANSWER 220 OF 249 REGISTRY COPYRIGHT 2004 ACS  
 RN 177570-32-0 REGISTRY  
 CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(2-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (*R*)- (9CI)  
 (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C<sub>22</sub>H<sub>21</sub>ClN<sub>4</sub>  
 SR CA  
 LC STN Files: CA, CAPLUS  
 Absolute stereochemistry.



\*\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

\*\*\*\*\*

L2 ANSWER 221 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 177499-41-1 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[(1*S*)-1-phenylethyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-(1-phenylethyl)-, (*S*)-

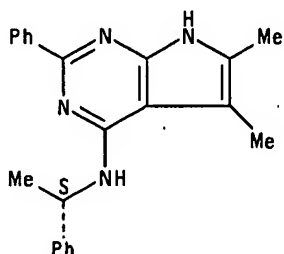
FS STEREOSEARCH

MF C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

REFERENCE 2:

125:25634

\*\*\*\*\*

L2 ANSWER 222 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 177499-40-0 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[(1*R*)-1-phenylethyl]-, (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-(1-phenylethyl)-; (*R*)-

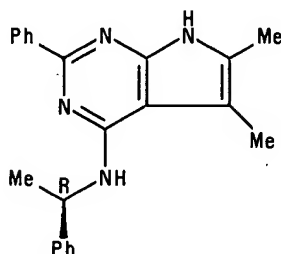
FS STEREOSEARCH

MF C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

REFERENCE 2:

131:281026

REFERENCE 3:

125:25634

\*\*\*\*\*

L2 ANSWER 223 OF 249 REGISTRY COPYRIGHT 2004 ACS

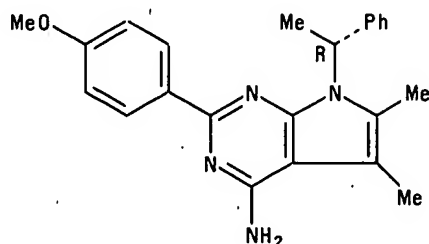
RN 177499-37-5 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(4-methoxyphenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (*R*)- (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C<sub>23</sub>H<sub>24</sub>N<sub>4</sub>O

SR CA

LC STN Files: CA, CAPLUS  
Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

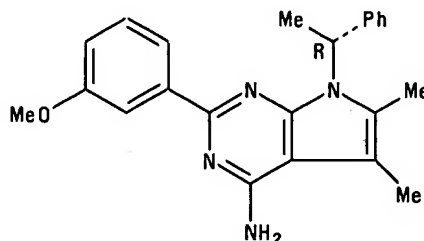
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

\*\*\*\*\*

L2 ANSWER 224 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 177499-36-4 REGISTRY  
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(3-methoxyphenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (*R*)- (9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C<sub>23</sub>H<sub>24</sub>N<sub>4</sub>O  
SR CA  
LC STN Files: CA, CAPLUS  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

\*\*\*\*\*

L2 ANSWER 225 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 177499-35-3 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(3,4-dichlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (S)- (9CI)  
(CA INDEX NAME)

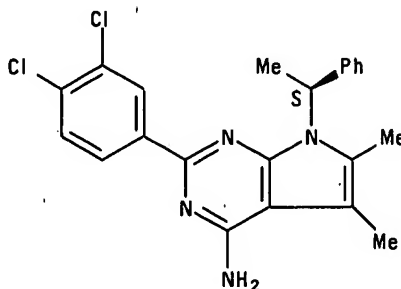
FS STEREOSEARCH

MF C<sub>22</sub>H<sub>20</sub>Cl<sub>2</sub>N<sub>4</sub>

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

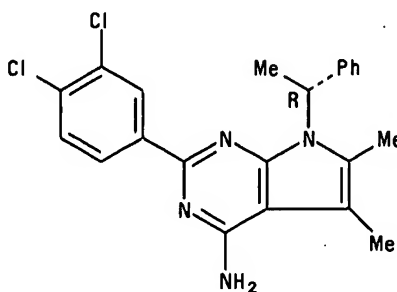
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

\*\*\*\*\*

L2 ANSWER 226 OF 249 REGISTRY COPYRIGHT 2004 ACS  
 RN 177499-34-2 REGISTRY  
 CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(3,4-dichlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (*R*)- (9CI)  
 (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C<sub>22</sub>H<sub>20</sub>Cl<sub>2</sub>N<sub>4</sub>  
 SR CA  
 LC STN Files: CA, CAPLUS  
 Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

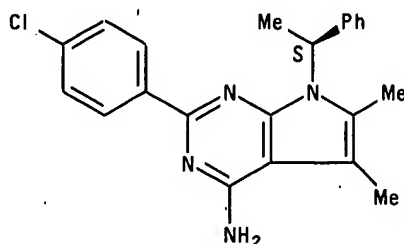
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

\*\*\*\*\*

L2 ANSWER 227 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 177499-33-1 REGISTRY  
CN 7H-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(4-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (S)- (9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C<sub>22</sub>H<sub>21</sub>ClN<sub>4</sub>  
SR CA  
LC STN Files: CA, CAPLUS  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

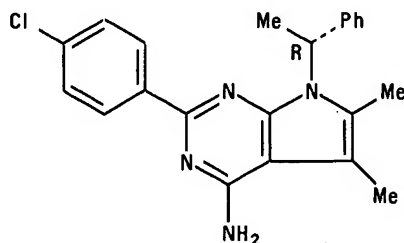
REFERENCE 1:

125:25634

\*\*\*\*\*



L2 ANSWER 228 OF 249 REGISTRY COPYRIGHT 2004 ACS  
 RN 177499-32-0 REGISTRY  
 CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(4-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (*R*)- (9CI)  
 (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C<sub>22</sub>H<sub>21</sub>ClN<sub>4</sub>  
 SR CA  
 LC STN Files: CA, CAPLUS  
 Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

\*\*\*\*\*

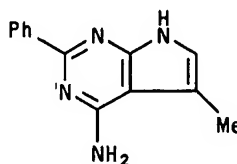
# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 280

L2 ANSWER 229 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 170170-17-9 REGISTRY  
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5-methyl-2-phenyl- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C<sub>13</sub>H<sub>12</sub>N<sub>4</sub>  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

123:313913

\*\*\*\*\*

L2 ANSWER 230 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 157838-12-5 REGISTRY

CN 7H-Pyrrolo[2,3-*d*]pyrimidin-4-amine,  
2-[4-[[[(10,11-dihydro-5*H*-dibenzo[*a,d*]cyclohepten-5-yl)methyl]amino]-1-piperidinyl]-*N*,7-di-2-propenyl-,  
(2*E*)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7H-Pyrrolo[2,3-*d*]pyrimidin-4-amine,  
2-[4-[[[(10,11-dihydro-5*H*-dibenzo[*a,d*]cyclohepten-5-yl)methyl]amino]-1-piperidinyl]-*N*,7-di-2-propenyl-,  
(*E*)-2-butenedioate (1:1)

FS STEREOSEARCH

MF C<sub>33</sub>H<sub>38</sub>N<sub>6</sub>.C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>

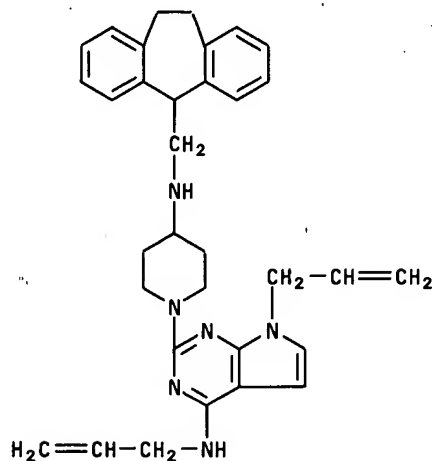
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

CM 1

CRN 157838-11-4

CMF C<sub>33</sub>H<sub>38</sub>N<sub>6</sub>

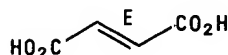


CM 2

CRN 110-17-8

CMF C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>

Double bond geometry as shown.



2 REFERENCES IN FILE CA (1907 TO DATE)

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 282

L2 ANSWER 230 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 157838-12-5 REGISTRY

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:237579

REFERENCE 2:

121:205381

\*\*\*\*\*  
L2 ANSWER 231 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 157838-11-4 REGISTRY

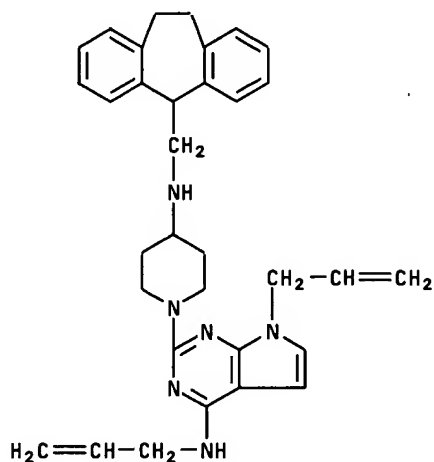
CN 7H-Pyrrolo[2,3-*d*]pyrimidin-4-amine,  
2-[4-[[[(10,11-dihydro-5H-dibenzo[*a,d*]cyclohepten-5-yl)methyl]amino]-1-piperidinyl]-N,7-di-2-propenyl-  
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>33</sub>H<sub>38</sub>N<sub>6</sub>

CI COM

SR CA



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 232 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 130147-83-0 REGISTRY

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(3-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(3-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (±)-

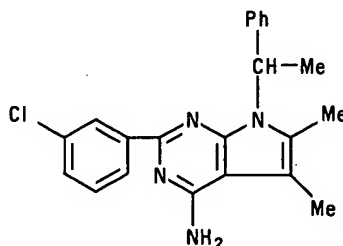
FS 3D CONCORD

MF C<sub>22</sub>H<sub>21</sub>ClN<sub>4</sub>

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

113:211696

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 284

L2 ANSWER 233 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 130147-82-9 REGISTRY

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(2-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(2-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (±)-

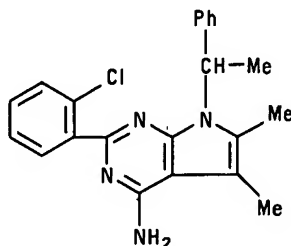
FS 3D CONCORD

MF C<sub>22</sub>H<sub>21</sub>ClN<sub>4</sub>

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

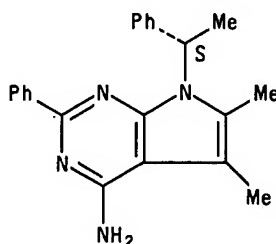
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

113:211696

\*\*\*\*\*

L2 ANSWER 234 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 130147-81-8 REGISTRY  
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-, (*S*)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)  
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

REFERENCE 2:

113:211696

\*\*\*\*\*

L2 ANSWER 235 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 130147-80-7 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-[(1*R*)-1-phenylethyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-, (*R*)-

FS STEREOSEARCH

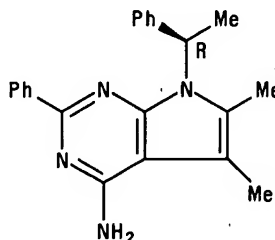
MF C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, USPAT2, USPATFULL

(\*File contains numerically searchable property data)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

REFERENCE 2:

130:71627

REFERENCE 3:

127:156859

REFERENCE 4:

125:157747

REFERENCE 5:

125:157746

REFERENCE 6:

125:25634



# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 287  
L2 ANSWER 235 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 130147-80-7 REGISTRY

REFERENCE 7:

113:211696

\*\*\*\*\*  
L2 ANSWER 236 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 130147-79-4 REGISTRY

CN 1H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(2-chlorophenyl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

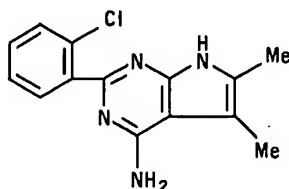
FS 3D CONCORD

MF C<sub>14</sub>H<sub>13</sub>ClN<sub>4</sub>

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

127:156859

REFERENCE 2:

113:211696

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 288

L2 ANSWER 237 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 130147-78-3 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(3-chlorophenyl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

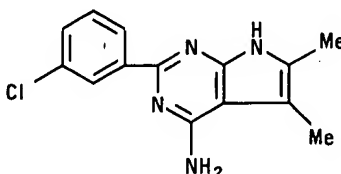
FS 3D CONCORD

MF C<sub>14</sub>H<sub>13</sub>ClN<sub>4</sub>

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

113:211696

\*\*\*\*\*

L2 ANSWER 238 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 116673-09-7 REGISTRY

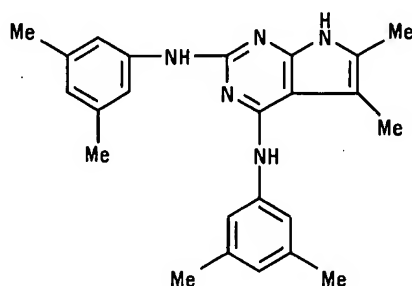
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidine-2,4-diamine, *N,N'*-bis(3,5-dimethylphenyl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>24</sub>H<sub>27</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT, SPECINFO



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

109:149471

\*\*\*\*\*

L2 ANSWER 239 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 116673-08-6 REGISTRY

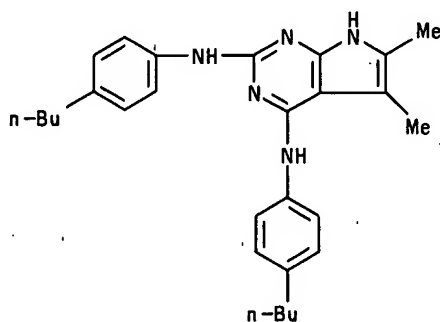
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidine-2,4-diamine, *N,N'*-bis(4-butylphenyl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>28</sub>H<sub>35</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT, SPECINFO



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

109:149471

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 291

L2 ANSWER 240 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 116673-07-5 REGISTRY

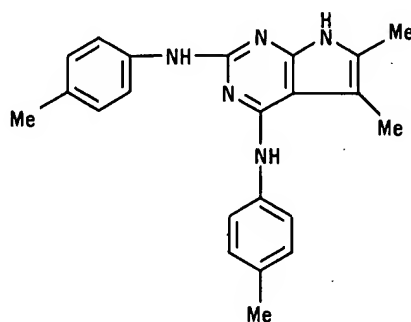
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidine-2,4-diamine, 5,6-dimethyl-*N,N'*-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>22</sub>H<sub>23</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT, SPECINFO



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

109:149471

\*\*\*\*\*

L2 ANSWER 241 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 116673-06-4 REGISTRY

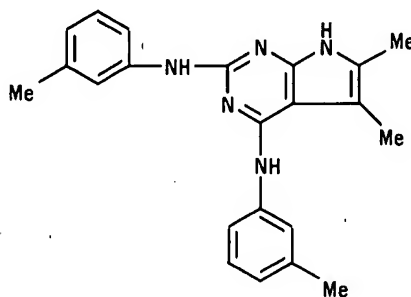
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidine-2,4-diamine, 5,6-dimethyl-*N,N'*-bis(3-methylphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>22</sub>H<sub>23</sub>N<sub>5</sub>

SR CA

LC STN Files: CA, CAPLUS, CASREACT, SPECINFO



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

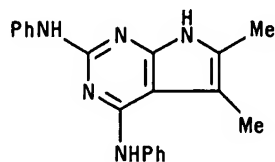
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

109:149471

\*\*\*\*\*

L2 ANSWER 242 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 116673-05-3 REGISTRY  
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidine-2,4-diamine, 5,6-dimethyl-*N,N'*-diphenyl- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C<sub>20</sub>H<sub>19</sub>N<sub>5</sub>  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT, SPECINFO



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

109:149471

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 294

L2 ANSWER 243 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 111601-40-2 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(4-chlorophenyl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

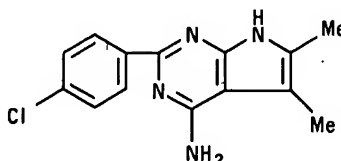
FS 3D CONCORD

MF C<sub>14</sub>H<sub>13</sub>ClN<sub>4</sub>

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT

(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

113:211696

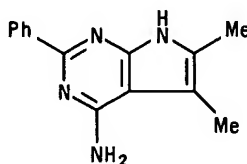
REFERENCE 2:

107:236656

\*\*\*\*\*



L2 ANSWER 244 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 111601-39-9 REGISTRY  
CN 1H-Pyrrolo[2,3-d]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C<sub>14</sub>H<sub>14</sub>N<sub>4</sub>  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

124:249637

REFERENCE 2:

113:211696

REFERENCE 3:

107:236656

\*\*\*\*\*

L2 ANSWER 245 OF 249 REGISTRY COPYRIGHT 2004 ACS

**RN 111601-37-7 REGISTRY**

CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(4-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)- (9CI) (CA INDEX NAME)

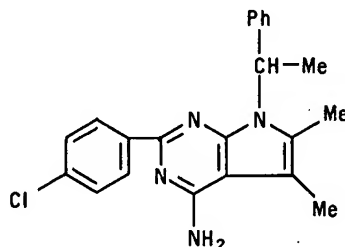
**FS      3D    CONCORD**

**MF** **C<sub>22</sub>H<sub>21</sub>ClN<sub>4</sub>**

**SR      CA**

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT

(\*File contains numerically searchable property data)



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

107:236656

.....

L2 ANSWER 246 OF 249 REGISTRY COPYRIGHT 2004 ACS

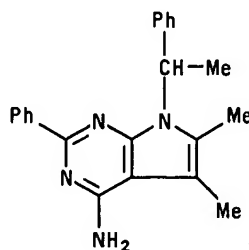
RN 111601-36-6 REGISTRY

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-(1-phenylethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

107:236656

\*\*\*\*\*

# STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 298

L2 ANSWER 247 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 94966-89-9 REGISTRY

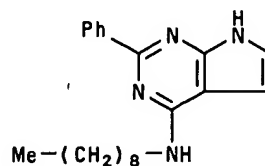
CN 7H-Pyrrolo[2,3-d]pyrimidine, 4-(nonylamino)-2-phenyl- (7CI) (CA INDEX NAME)

FS 3D CONCORD

MF C<sub>21</sub>H<sub>28</sub>N<sub>4</sub>

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, TOXCENTER

(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

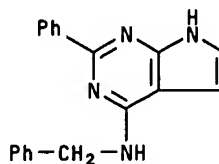
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1:

57:76026

\*\*\*\*\*

L2 ANSWER 248 OF 249 REGISTRY COPYRIGHT 2004 ACS  
RN 94304-61-7 REGISTRY  
CN 7H-Pyrrolo[2,3-d]pyrimidine, 4-(benzylamino)-2-phenyl- (7CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C<sub>19</sub>H<sub>16</sub>N<sub>4</sub>  
LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS  
(\*File contains numerically searchable property data).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

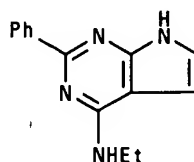
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1:

56:46024

\*\*\*\*\*

L2 ANSWER 249 OF 249 REGISTRY COPYRIGHT 2004 ACS  
 RN 92193-06-1 REGISTRY  
 CN 7H-Pyrrolo[2,3-d]pyrimidine, 4-(ethylamino)-2-phenyl- (7CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C<sub>14</sub>H<sub>14</sub>N<sub>4</sub>  
 LC STN Files: CA, CAOLD, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1:

56:46024

\*\*\*\*\*

E0490133

2004 077 14:28:54

REQUEST NUMBER: P077139C

BEVERLY SHEARS  
US PATENT & TRADEMARK OFFICE  
BIOTECH/CHEM LIBRARY, RM 1A54  
HENRY REMSEN, JR. BLDG.  
400 DULANY ST.  
ALEXANDRIA, VA 22314

File HCAPlus e 30 ans.

## CHEMICAL ABSTRACTS "HCAplus FILE"

The HCAplus File contains records for all articles from nearly 1,500 key chemical journals since October, 1994, as well as the documents selected for coverage or covered in Chemical Abstracts for the time period 1907-present.

Copies of most original documents may be obtained from the CAS Document Detective Service (CAS DDS).

The field codes that you may see in this offline print are listed below.

## Display

Code	Definition
------	------------

-----	-----
-------	-------

AN	Accession Number
DN	Document Number (CA Abstract Number)
OREF	Original Reference Number
ED	Entry Date
TI	Title of Document
AU	Author
IN	Patent Inventor
CS	Corporate Source
PA	Patent Assignee
SO	Source
JT	Journal Title
PB	Publisher
PUI	Publisher Item Identifier
URL	Uniform Resource Locator
DT	Document Type
LA	Language
IC	International Patent Classification (IPC)
ICM	Main IPC
ICS	Secondary IPC
ICA	Additional or Supplementary IPC
ICI	Index or Complementary IPC
NCL	National Patent Classification Code
CC	Classification Code (CA Section Code and Title and



CA Section Cross-Reference Code)

FAN.CNT	Family Accession Number Count
CY.CNT	Patent Country Count
PN.CNT	Patent Number Count
PI	Patent Information or Patent Family Table
DS	Designated States (patent)
AI	Patent Application Information
PRAI	Priority Application Information
PY	Publication Year
FAN	Family Accession Number
OS	Other Source
GI	Graphic Image
AB	Abstract
ST	Supplementary Term (CA Keywords)
IT	Index Term
RL	Role
REC.CNT	Cited References Count
RE	Cited References
RETABLE	Cited References Table

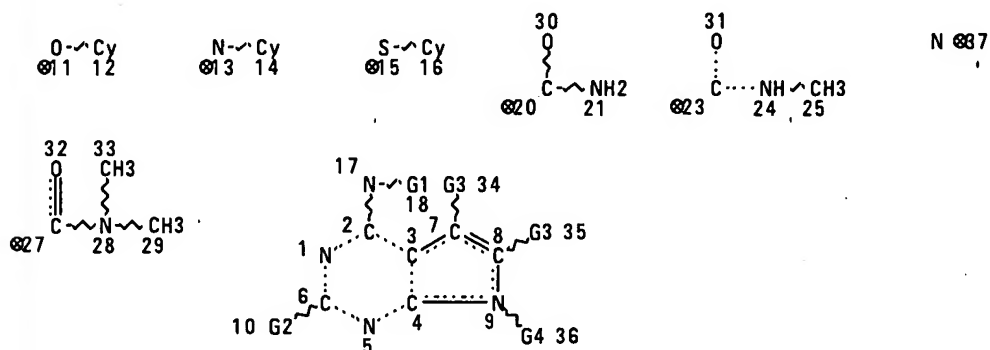
# STN INTERNATIONAL®

HCAPLUS FILE SEARCH STATISTICS - P077139C

17 MAR 2004 20:04:18 PAGE 3

30 ANSWERS PRINTED IN FORMAT 'ED IBIB ABS HITRN'  
IN FILE 'HCAPLUS'  
USING QUERY:

L1 STR



VAR G1=H/CH3/20/23/27

VAR G2=11/13/15/CY

VAR G3=H/CH3

VAR G4=C/37/H

NODE ATTRIBUTES:

NSPEC IS R AT 37

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L2 249 SEA FILE=REGISTRY SSS FUL L1

L3 30 SEA FILE=HCAPLUS L2

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

4

L3 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 04 Feb 2004

ACCESSION NUMBER: 2004:88297 HCAPLUS

DOCUMENT NUMBER: 140:146159

TITLE: Preparation and use of substituted pyrrolo[2,3-d]pyrimidines as selective adenosine A<sub>3</sub> receptor antagonists

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: U.S., 71 pp., Cont.-in-part of Appl. No. PCT/US99/12135.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6686366	B1	20040203	US 1999-454075	19991202
WO 9962518	A1	19991209	WO 1999-US12135	19990601

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

WO 2001039777	A1	20010607	WO 2000-US32702	20001201
---------------	----	----------	-----------------	----------

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1246623	A1	20021009	EP 2000-988011	20001201
------------	----	----------	----------------	----------

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

L3 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2004 ACS

JP 2003519102

T2

20030617

JP 2001-541509

20001201

PRIORITY APPLN. INFO.:

US 1998-87702P P 19980602

US 1999-123216P P 19990308

US 1999-126527P P 19990326

WO 1999-US12135 A2 19990601

US 1999-454074 A 19991202

US 1999-454075 A 19991202

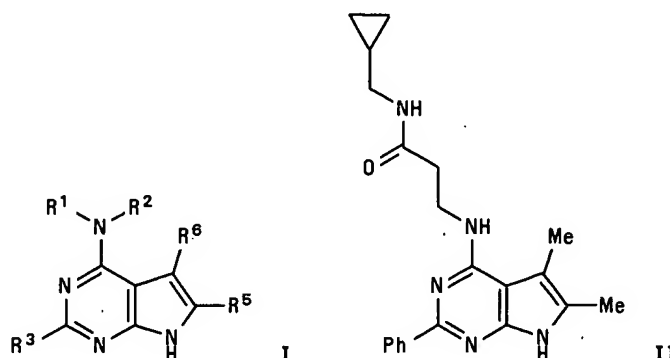
US 1999-454254 A 19991202

WO 2000-US32702 W 20001201

OTHER SOURCE(S):

MARPAT 140:146159

GI



**AB** The title compds. [I; R<sup>1</sup> = H and R<sup>2</sup> = cyclopropylmethylaminocarbonylethyl, cis-3-hydroxycyclopentyl, acetamidobutyl, etc.; or NR<sup>1</sup>R<sup>2</sup> = 3-acetamidopiperadino, 3-hydroxypyrrolidino, 3-methoxycarbonylmethylpyrrolidino, etc.; R<sup>3</sup> = (un)substituted cycloalkyl, aryl; R<sup>5</sup> = H, alkyl, aryl; R<sup>6</sup> = H, alkyl, cycloalkyl] which specifically inhibit the adenosine A<sub>3</sub> receptor and are useful for treating a disease assocd. with A<sub>3</sub> adenosine receptor, were prepd. Thus, 4-chloro-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine was reacted with 4-trans-hydroxycyclohexylamine in DMSO at 130°C for 5 h to yield I [R<sup>1</sup> = H; R<sup>2</sup> = trans-4-hydroxycyclohexyl; R<sup>3</sup> = Ph; R<sup>5</sup>, R<sup>6</sup> = Me] in 75% yield after purifn. which showed K<sub>i</sub> of 13.9 nM against adenosine receptor A<sub>1</sub> binding. Some of the compds. I such as II exhibited at least 10 times more selective binding to adenosine receptor A<sub>3</sub> than other receptor subtype. Claimed uses of I includes administration of a systemic formulation (i.e. ophthalmic) for the treatment of a disease assocd. with A<sub>3</sub> adenosine receptors in a subject.

**IT** \*\*\*251946-19-7P\*\*\*

RL: BYP (Byproduct); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant)

L3 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2004 ACS

or reagent); USES (Uses)

(prepn. and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as selective adenosine A<sub>3</sub> receptor antagonists)

IT \*\*\*251946-18-6P\*\*\*

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as selective adenosine A<sub>3</sub> receptor antagonists)

IT ***246855-41-4P***	***246855-42-5P***	***251945-90-1P***
***251945-91-2P***	***251945-92-3P***	***251945-93-4P***
***251945-94-5P***	***251945-95-6P***	***251945-96-7P***
***251945-97-8P***	***251945-98-9P***	***251945-99-0P***
***251946-00-6P***	***251946-01-7P***	***251946-03-9P***
***251946-04-0P***	***251946-05-1P***	***251946-06-2P***
***251946-07-3P***	***251946-08-4P***	***251946-09-5P***
***251946-10-8P***	***251946-11-9P***	***251946-12-0P***
***251946-13-1P***	***251946-14-2P***	***251946-15-3P***
***251946-16-4P***	***251946-17-5P***	***251946-20-0P***
***251946-21-1P***	***251946-22-2P***	***251946-23-3P***
***251946-24-4P***	***251946-25-5P***	***251946-26-6P***
***251946-27-7P***	***251946-28-8P***	***251946-29-9P***
***251946-30-2P***	***251946-31-3P***	***251946-32-4P***
***251946-33-5P***	***251946-34-6P***	***251946-35-7P***
***251946-36-8P***	***251946-37-9P***	***251946-38-0P***
***251946-39-1P***	***251946-40-4P***	***251946-41-5P***
***251946-42-6P***	***251946-43-7P***	***251946-44-8P***
***251946-45-9P***	***251946-46-0P***	***251946-47-1P***
***251946-48-2P***	***251946-49-3P***	***251946-50-6P***
***251946-52-8P***	***251946-54-0P***	***251946-55-1P***
***251946-56-2P***	***251946-57-3P***	***251946-58-4P***
***251946-59-5P***	***251947-22-5P***	***251947-24-7P***
***343631-95-8P***	***343631-96-9P***	***343631-97-0P***
***343631-99-2P***	***343632-03-1P***	***343632-04-2P***
***343632-05-3P***	***343632-06-4P***	***343632-07-5P***
***343632-08-6P***	***343632-09-7P***	***343632-10-0P***
***343632-11-1P***	***343632-12-2P***	***343632-13-3P***
***343632-14-4P***	***343632-15-5P***	***343632-31-5P***
***343632-32-6P***	***343632-33-7P***	***343632-35-9P***
***343632-36-0P***	***343632-37-1P***	***343632-38-2P***

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

7

L3 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2004 ACS

\*\*\*343632-50-8P\*\*\*      \*\*\*343632-70-2P\*\*\*      \*\*\*343632-71-3P\*\*\*

\*\*\*343632-72-4P\*\*\*      \*\*\*343632-73-5P\*\*\*      \*\*\*343632-77-9P\*\*\*

\*\*\*343632-78-0P\*\*\*      \*\*\*343632-79-1P\*\*\*      \*\*\*343633-16-9P\*\*\*

\*\*\*343969-79-9P\*\*\*      \*\*\*343969-97-1P\*\*\*

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as selective adenosine A<sub>3</sub> receptor antagonists)

IT      \*\*\*343632-96-2P\*\*\*      \*\*\*343632-97-3P\*\*\*

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as selective adenosine A<sub>3</sub> receptor antagonists)

REFERENCE COUNT:      128      THERE ARE 128 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

\*\*\*\*\*

L3 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 25 Jul 2003

ACCESSION NUMBER: 2003:570644 HCAPLUS

DOCUMENT NUMBER: 139:133575

TITLE: Preparation of bicyclic pyrimidinyl derivatives as adenosine receptor ligands

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan

PATENT ASSIGNEE(S): OSI Pharmaceuticals Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 105 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

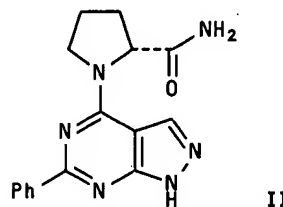
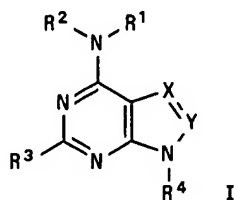
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003139427	A1	20030724	US 2002-227378	20020823
PRIORITY APPLN. INFO.:			US 2002-227378	20020823

OTHER SOURCE(S): MARPAT 139:133575

GI



AB Title compds. I [Y = N, CR<sup>5</sup> and X = N, CR<sup>6</sup> wherein X, Y are both N or when Y = CR<sup>5</sup>, X = N or when X = CR<sup>6</sup>, Y = N; R<sup>1-2</sup> = H, alkoxy, aminoalkyl, etc; R<sup>3-4</sup> = H, alkyl, aryl, alkylaryl] are prepd. For instance, 3-amino-4-carbamoylpyrazole is acylated with benzoyl chloride (Pyridine, 50°, 5-6 h), cyclized to the corresponding pyrazolopyrimidine (water, K<sub>2</sub>CO<sub>3</sub>, 100°, 16 h), converted to the chloride (POCl<sub>3</sub>, 106°, 2 h) and used for reactions with various amines to give the example compds., e.g., II. II has K<sub>i</sub> = 76.7 nM for the adenosine A1 receptor, K<sub>i</sub> = 242.7 nM for A2a and K<sub>i</sub> = 1480.5 nM for A2b. I are useful for the treatment of.

IT ***246855-41-4P***	***246855-42-5P***	***251945-90-1P***
***251945-91-2P***	***251945-92-3P***	***251945-93-4P***
***251945-94-5P***	***251945-95-6P***	***251945-96-7P***

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

9

L3 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2004 ACS

***251945-97-8P***	***251945-98-9P***	***251945-99-0P***
***251946-00-6P***	***251946-01-7P***	***251946-03-9P***
***251946-06-2P***	***251946-07-3P***	***251946-08-4P***
***251946-10-8P***	***251946-11-9P***	***251946-12-0P***
***251946-13-1P***	***251946-14-2P***	***251946-15-3P***
***251946-16-4P***	***251946-17-5P***	***251946-19-7P***
***251946-20-0P***	***251946-21-1P***	***251946-22-2P***
***251946-23-3P***	***251946-24-4P***	***251946-26-6P***
***251946-27-7P***	***251946-28-8P***	***251946-29-9P***
***251946-30-2P***	***251946-31-3P***	***251946-32-4P***
***251946-33-5P***	***251946-34-6P***	***251946-35-7P***
***251946-36-8P***	***251946-37-9P***	***251946-38-0P***
***251946-39-1P***	***251946-40-4P***	***251946-41-5P***
***251946-42-6P***	***251946-44-8P***	***251946-45-9P***
***251946-46-0P***	***251946-47-1P***	***251946-48-2P***
***251946-49-3P***	***251946-50-6P***	***251946-57-3P***
***251946-58-4P***	***251946-59-5P***	***251947-22-5P***
***251947-24-7P***	***343632-03-1P***	***343632-04-2P***
***343632-05-3P***	***343632-06-4P***	***343632-07-5P***
***343632-08-6P***	***343632-09-7P***	***343632-10-0P***
***343632-11-1P***	***343632-12-2P***	***343632-13-3P***
***343632-14-4P***	***343632-15-5P***	***343632-16-6P***
***343632-17-7P***	***343632-19-9P***	***343632-20-2P***
***343632-21-3P***	***343632-31-5P***	***343632-32-6P***
***343632-33-7P***	***343632-35-9P***	***343632-36-0P***
***343632-37-1P***	***343632-38-2P***	***343632-50-8P***
***343969-79-9P***	***343969-97-1P***	***443118-43-2P***
***443118-44-3P***	***443118-78-3P***	***443760-82-5P***
***565234-92-6P***		

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of bicyclic pyrazolo- imidazo- and triazolopyrimidinyl derivs. as adenosine receptor ligands)

\*\*\*\*\*



# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

10

L3 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 04 Jul 2003

ACCESSION NUMBER: 2003:511094 HCAPLUS

DOCUMENT NUMBER: 139:85365

TITLE: Preparation of pyrrolopyrimidine A<sub>2b</sub> selective antagonist compounds,  
method of synthesis and therapeutic use

INVENTOR(S): Castelhana, Arlindo L.; Mckibben, Bryan; Steinig, Arno G.

PATENT ASSIGNEE(S): Osi Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 223 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053361	A2	20030703	WO 2002-US40890	20021220

WO 2003053361	A3	20031224		
---------------	----	----------	--	--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR,  
CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID,  
IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,  
MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG,  
SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW,  
AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY,  
CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK,  
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003229067	A1	20031211	US 2002-326005	20021220
---------------	----	----------	----------------	----------

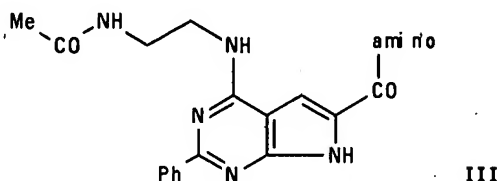
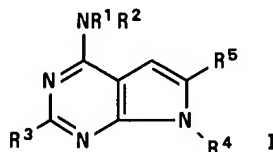
PRIORITY APPLN. INFO.:

US 2001-343443P P 20011220

OTHER SOURCE(S): CASREACT 139:85365; MARPAT 139:85365

GI

L3 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2004 ACS



AB The subject invention provides pyrrolopyrimidines (shown as I; see below for variable definitions; e.g.  
 N-[2-[6-[1-[2-(2-chlorophenyl)ethyl]piperidin-4-yloxymethyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl-amino]ethyl]acetamide (II)) or a specific enantiomer thereof, or a specific tautomer thereof, or a pharmaceutically acceptable salt thereof, and a method for treating a disease assocd. with the A<sub>2b</sub> adenosine receptor. For I: R<sup>1</sup> is a (un)substituted alkyl (substituent = hydroxyl, dihydroxy, carboxyl, -C(O)NR<sup>a</sup>R<sup>b</sup>, -NR<sup>a</sup>R<sup>b</sup>, -NR<sup>a</sup>C(O)NR<sup>a</sup>R<sup>b</sup>, -NR<sup>a</sup>C(O)OR<sup>a</sup>, -OC(O)NR<sup>a</sup>R<sup>b</sup>, or -NHC(O)R<sup>a</sup>). R<sup>2</sup> is H or a (un)substituted alkyl (substituent = hydroxyl, dihydroxy, carboxyl, -C(O)NR<sup>a</sup>R<sup>b</sup>, -NR<sup>a</sup>R<sup>b</sup>, -NR<sup>a</sup>C(O)NR<sup>a</sup>R<sup>b</sup>, -NR<sup>a</sup>C(O)OR<sup>a</sup>, -OC(O)NR<sup>a</sup>R<sup>b</sup>, or -NHC(O)R<sup>a</sup>), or R<sup>1</sup>, R<sup>2</sup> and N together form a substituted piperazine, substituted azetidine, or a pyrrolidine ring substituted with -(CH<sub>2</sub>)<sub>2</sub>OH or -CH<sub>2</sub>C(O)OH. R<sup>3</sup> is a (un)substituted Ph or a 5-6 membered heteroaryl ring, wherein the substituent is halogen, hydroxyl, cyano, (C<sub>1</sub>-C<sub>15</sub>)alkyl, (C<sub>1</sub>-C<sub>15</sub>)alkoxyl or -NR<sup>a</sup>R<sup>b</sup>; R<sup>4</sup> is H or (un)substituted (C<sub>1</sub>-C<sub>15</sub>)alkyl; R<sup>5</sup> is -(CH<sub>2</sub>)<sub>m</sub>OR<sup>6</sup>, -CHNOR<sup>7</sup>, -C(O)NR<sup>8</sup>R<sup>9</sup>, -(CH<sub>2</sub>)<sub>m</sub>C(O)OR<sup>10</sup>, -(CH<sub>2</sub>)<sub>k</sub>C(O)NR<sup>11</sup>R<sup>12</sup>; addnl. details are given in the claims. Radioligand binding assays yielded selectivities for the A<sub>2b</sub> receptor relative to the A<sub>1</sub>, A<sub>2a</sub> and A<sub>3</sub> receptors for 9 examples of I, e.g. 26 times for II. About 26 example preps. of I and intermediates and characterization data for hundreds of I and intermediates are included. For example, III can be prepd. by reacting 4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine with PhSO<sub>2</sub>Cl and a reducing agent in the presence of solvent to produce 7-benzenesulfonyl-4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine, which was reacted with CO<sub>2</sub> in the presence of LDA and a solvent to produce lithium 7-benzenesulfonyl-4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine-6-carboxylate, which was reacted with AcNHCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> in the presence of solvent to give 4-(2-acetylaminoethylamino)-7-benzenesulfonyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, which was deprotected with a hydroxide base and subsequently condensed with amines.

IT \*\*\*553634-53-0P\*\*\*

N-[2-[[6-Methyl-7-[2-oxo-2-[4-(3-phenylallyl)piperazin-1-yl]ethyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimi-

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

12

L3 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2004 ACS

din-4-yl]amino]ethyl]acetamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; prepn. of pyrrolopyrimidine A<sub>2b</sub> selective antagonist compds., method of synthesis and therapeutic use)

\*\*\*\*\*

L3 ANSWER 4 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 13 Jun 2003

ACCESSION NUMBER: 2003:454286 HCAPLUS

DOCUMENT NUMBER: 139:36534

TITLE: Preparation of arylpyrrolopyrimidines as adenosine A<sub>1</sub> and A<sub>3</sub> receptor inhibitors

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Werner, Douglas S.; Witter, David

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 170 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003048120	A2	20030612	WO 2002-US38055	20021127
WO 2003048120	A3	20030904		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

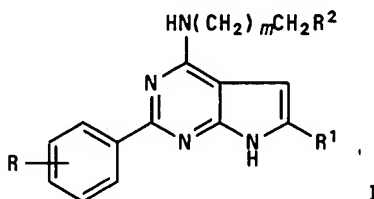
PRIORITY APPLN. INFO.:

US 2001-335273P P 20011130

US 2001-337274P P 20011130

OTHER SOURCE(S): MARPAT 139:36534

L3 ANSWER 4 OF 30 HCAPLUS COPYRIGHT 2004 ACS  
GI



AB Arylpyrrolopyrimidines I [ $m = 0-3$ ;  $R =$  halogen, alkyl, alkoxy, OH,  $\text{NH}_2$ , alkylamino;  $R^1 =$  H, (un)substituted alkyl, aryl, aralkyl;  $R^2 =$  (un)substituted imidazole, pyrazole, attached through C] which specifically inhibit the adenosine  $A_1$  and  $A_3$  receptors were prep'd. Thus, 4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine was treated with histamine to give the 4-[2-(1H-imidazol-2-yl)ethyl]amino analog which had  $A_3$  inhibiting activity  $\geq 10$  times greater than that of ref. compds.

IT \*\*\*541503-67-7P\*\*\*      \*\*\*541503-83-7P\*\*\*      \*\*\*541503-85-9P\*\*\*  
\*\*\*541503-91-7P\*\*\*

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of arylpyrrolopyrimidines as adenosine  $A_1$  and  $A_3$  receptor inhibitors)

IT \*\*\*251946-11-9P\*\*\*      \*\*\*251947-22-5P\*\*\*      \*\*\*251947-24-7P\*\*\*  
\*\*\*343632-31-5P\*\*\*      \*\*\*343632-32-6P\*\*\*      \*\*\*343632-33-7P\*\*\*  
\*\*\*343632-35-9P\*\*\*      \*\*\*343632-36-0P\*\*\*      \*\*\*343632-37-1P\*\*\*  
\*\*\*343632-38-2P\*\*\*      \*\*\*343632-50-8P\*\*\*      \*\*\*443118-47-6P\*\*\*  
\*\*\*541503-35-9P\*\*\*      \*\*\*541503-69-9P\*\*\*      \*\*\*541503-71-3P\*\*\*  
\*\*\*541503-73-5P\*\*\*      \*\*\*541503-75-7P\*\*\*      \*\*\*541503-77-9P\*\*\*  
\*\*\*541503-80-4P\*\*\*      \*\*\*541503-87-1P\*\*\*

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of arylpyrrolopyrimidines as adenosine  $A_1$  and  $A_3$  receptor inhibitors)

\*\*\*\*\*

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

14

L3 ANSWER 5 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 18 Apr 2003

ACCESSION NUMBER: 2003:300617 HCAPLUS

DOCUMENT NUMBER: 138:321287

TITLE: Preparation of deazapurines as adenosine A<sub>3</sub> receptor antagonists.

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 77 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
US 2003073708	A1	20030417	US 2001-6405	20011130
US 6673802	B2	20040106		

PRIORITY APPLN. INFO.:

US 2000-250748P P 20001201

OTHER SOURCE(S): MARPAT 138:321287

GI



AB Title compds. [I; R<sup>1</sup>, R<sup>2</sup> = H, (substituted) alkyl, aryl, aralkyl; R<sup>1</sup>R<sup>2</sup> = atoms to form (substituted) heterocyclyl; R<sup>3</sup> = (substituted) alkyl, aryl, aralkyl; R<sup>4</sup> = H, (substituted) alkyl, aryl, aralkyl; R<sup>5</sup>, R<sup>6</sup> = H, halo, (substituted) alkyl, aryl, alkylaryl; R<sup>4</sup>R<sup>5</sup> or R<sup>5</sup>R<sup>6</sup> = (substituted) heterocyclyl, carbocyclyl], were prepd. Thus, 2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-ylamine and histamine were heated at 120° in Me<sub>2</sub>SO for 6.5 h to give 43% [2-(3H-imidazol-4-yl)ethyl] [2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amine. The latter had 10 times the A<sub>3</sub> receptor binding affinity of a ref. compd.

IT \*\*\*443118-47-6P\*\*\*

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compd.; prepn. of deazapurines as adenosine A<sub>3</sub> receptor antagonists)

IT \*\*\*246855-41-4P\*\*\*

\*\*\*246855-42-5P\*\*\*

\*\*\*251945-90-1P\*\*\*

\*\*\*251945-91-2P\*\*\*

\*\*\*251945-92-3P\*\*\*

\*\*\*251945-93-4P\*\*\*

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

15

L3 ANSWER 5 OF 30 HCAPLUS COPYRIGHT 2004 ACS

***251945-94-5P***	***251945-95-6P***	***251945-96-7P***
***251945-97-8P***	***251945-98-9P***	***251945-99-0P***
***251946-00-6P***	***251946-01-7P***	***251946-04-0P***
***251946-05-1P***	***251946-06-2P***	***251946-07-3P***
***251946-08-4P***	***251946-09-5P***	***251946-10-8P***
***251946-11-9P***	***251946-12-0P***	***251946-13-1P***
***251946-14-2P***	***251946-15-3P***	***251946-16-4P***
***251946-17-5P***	***251946-18-6P***	***251946-19-7P***
***251946-20-0P***	***251946-21-1P***	***251946-22-2P***
***251946-23-3P***	***251946-24-4P***	***251946-25-5P***
***251946-26-6P***	***251946-27-7P***	***251946-28-8P***
***251946-29-9P***	***251946-30-2P***	***251946-31-3P***
***251946-32-4P***	***251946-33-5P***	***251946-34-6P***
***251946-35-7P***	***251946-36-8P***	***251946-37-9P***
***251946-38-0P***	***251946-39-1P***	***251946-40-4P***
***251946-41-5P***	***251946-42-6P***	***251946-43-7P***
***251946-44-8P***	***251946-45-9P***	***251946-46-0P***
***251946-47-1P***	***251946-48-2P***	***251946-54-0P***
***251946-55-1P***	***251946-56-2P***	***251946-57-3P***
***251946-58-4P***	***251946-59-5P***	***343632-17-7P***
***343632-31-5P***	***343632-32-6P***	***343632-35-9P***
***343632-37-1P***	***343632-38-2P***	***343632-50-8P***
***500736-03-8P***	***512848-47-4P***	***512848-48-5P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of deazapurines as adenosine A<sub>3</sub> receptor antagonists)

IT \*\*\*343631-96-9\*\*\*

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of deazapurines as adenosine A<sub>3</sub> receptor antagonists)

IT \*\*\*251947-22-5P\*\*\* \*\*\*251947-24-7P\*\*\*

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of deazapurines as adenosine A<sub>3</sub> receptor antagonists)

\*\*\*\*\*

L3 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 07 Mar 2003

ACCESSION NUMBER: 2003:174478 HCAPLUS

DOCUMENT NUMBER: 138:221598

 TITLE: Preparation of pyrrolo[2,3-d]pyrimidinamines as selective adenosine A<sub>1</sub> receptor inhibitors for treatment of asthma, COPD, and other conditions

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 79 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

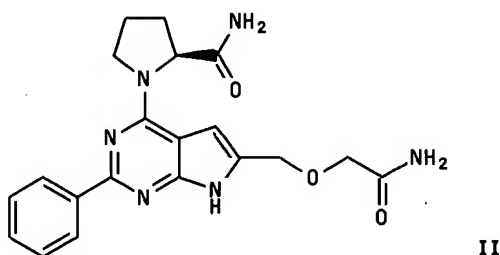
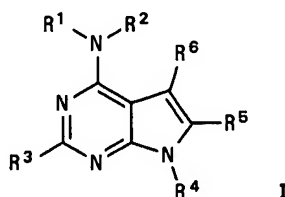
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003045536	A1	20030306	US 2001-280	20011130
US 6680324	B2	20040120		

PRIORITY APPLN. INFO.:

US 2000-250895P P 20001201

OTHER SOURCE(S): MARPAT 138:221598

GI



AB Title diazapurinamines I [wherein R<sup>1</sup>, R<sup>2</sup>, and R<sup>4</sup> = independently H or (un)substituted alkyl(aryl) or aryl; or NR<sup>1</sup>R<sup>2</sup> = (un)substituted heterocyclyl; R<sup>3</sup> = (un)substituted alkyl(aryl), aryl,

## L3 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2004 ACS

CO<sub>2</sub>H, carboxy esters, or carboxamides; or C<sub>2</sub>R<sup>3</sup>R<sup>4</sup> or C<sub>2</sub>R<sup>5</sup>R<sup>6</sup> = (un)substituted carbocyclyl or heterocyclyl; R<sup>5</sup> and R<sup>6</sup> = independently H, halo, or (un)substituted alkyl(aryl) or aryl; and pharmaceutically acceptable salts and prodrugs thereof] were prep'd. as adenosine A<sub>1</sub> specific inhibitors. For example, 4-chloro-5-methyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidine was protected with di-*t*-Bu dicarbonate (80%), brominated (84%), coupled with anhyd. Me glycolate (99%), coupled with L-prolinamide (92%), and deprotected (93%) to give II. The latter exhibited adenosine A<sub>1</sub> receptor binding equal to or surpassing that of ref. compds. and is expected to have better water soly. (cLogP = 1.5) than ref. compds. (cLogP = 3.8). Efficacy and structure activity profiles of diazapurines of the invention are also disclosed. Thus, I are useful for the treatment of asthma, chronic obstructive pulmonary disease (COPD), allergic rhinitis, upper respiratory disorder, and congestive heart failure (no data).

IT \*\*\*246855-41-4P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-08-4P\*\*\*

\*\*\*251946-14-2P\*\*\*

4-[(3-*tert*-Butyloxy-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-15-3P\*\*\*

4-[(2-Hydroxyethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-18-6P\*\*\*

4-[(4-*cis*-Benzoyloxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-24-4P\*\*\*

4-[(3-Hydroxy-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-31-3P\*\*\*

4-[(2-Aminoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-42-6P\*\*\*

4-[[1-Methyl-2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES

(Uses)

(A<sub>1</sub> receptor inhibitor; prepn. of pyrrolopyrimidinamines adenosine A<sub>1</sub> receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)

IT \*\*\*246855-42-5P\*\*\*

4-[(2-Acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251945-90-1P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-6-methyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251945-91-2P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5-methyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251945-92-3P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251945-93-4P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-pyridyl)-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251945-94-5P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-furyl)-7H-pyrrolo[2,3-*d*]pyrimidine



L3 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2004 ACS

\*\*\*251945-95-6P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-furyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251945-96-7P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-cyclopentyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251945-97-8P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-thienyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251945-98-9P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-thienyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251945-99-0P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(4-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-00-6P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-01-7P\*\*\*

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-03-9P\*\*\*

\*\*\*251946-06-2P\*\*\*

4-[(2-*trans*-Hydroxycyclopentyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-07-3P\*\*\*

4-[(3-*trans*-Hydroxycyclopentyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-10-8P\*\*\*

4-[(3-Amino-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-11-9P\*\*\*

4-[[3-(Cyclopropylmethylamino)-3-oxopropyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-12-0P\*\*\*

4-[(2-Amino-2-oxoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-13-1P\*\*\*

4-[[2-(Methylamino)-2-oxoethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-16-4P\*\*\*

4-[(3-Hydroxypropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-17-5P\*\*\*

4-[(4-Hydroxybutyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-19-7P\*\*\*

4-[(3-Cyclohexenyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-20-0P\*\*\*

4-[(4-*cis*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-21-1P\*\*\*

4-[[3-(Dimethylamino)-3-oxopropyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-22-2P\*\*\*

4-[(2-Formylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-23-3P\*\*\*

4-[(3-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-25-5P\*\*\*

4-[(3-Aminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-26-6P\*\*\*

L3 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2004 ACS

4-[[3-(Methylamino)-3-oxopropyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-27-7P\*\*\*

4-[[2-[(Cyclopropanecarbonyl)amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-28-8P\*\*\*

4-[(2-Isobutyrylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-29-9P\*\*\*

4-[(3-Propionylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-30-2P\*\*\*

4-[[2-(Methylsulfonylamino)ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-32-4P\*\*\*

4-[(2-Propionylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-33-5P\*\*\*

4-[[2-(*N*'-Methylureido)ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-34-6P\*\*\*

4-[[2-(*N*'-Ethylureido)ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-35-7P\*\*\*

4-[(2-Pyruvylamidoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine\*\*\*251946-36-8P\*\*\* 4-[(2-Ureidoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-37-9P\*\*\*

4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-38-0P\*\*\*

(R)-4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-39-1P\*\*\*

(R)-4-[(1-Methyl-2-acetylaminooethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-40-4P\*\*\*

(S)-4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-41-5P\*\*\*

(S)-4-[(1-Methyl-2-acetylaminooethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-44-8P\*\*\*

(S,S)-4-[(2-Acetylaminocyclohexyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-45-9P\*\*\*

4-[(2-Methyl-2-acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-46-0P\*\*\*

4-[(1-Methyl-2-acetylaminooethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-47-1P\*\*\*

(R,R)-4-[(2-Acetylaminocyclohexyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-48-2P\*\*\*

4-[(2-Acetyloxyethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-49-3P\*\*\*

\*\*\*251946-50-6P\*\*\*

\*\*\*251946-54-0P\*\*\*

4-[[2-(*N*'-Methylureido)propyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

L3 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2004 ACS

\*\*\*251946-55-1P\*\*\*

4-[(2-Acetamidobutyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-56-2P\*\*\*

4-[[2-(*N*'-Methylureido)butyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-57-3P\*\*\*

4-[(*trans*-4-Hydroxycyclohexyl)amino]-2-(3-chlorophenyl)-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-58-4P\*\*\*

4-[(*trans*-4-Hydroxycyclohexyl)amino]-2-(3-fluorophenyl)-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*251946-59-5P\*\*\*

\*\*\*251947-22-5P\*\*\*

\*\*\*251947-24-7P\*\*\*

\*\*\*343632-03-1P\*\*\*

\*\*\*343632-04-2P\*\*\*

\*\*\*343632-05-3P\*\*\*

\*\*\*343632-07-5P\*\*\*

\*\*\*343632-08-6P\*\*\*

\*\*\*343632-09-7P\*\*\*

\*\*\*343632-10-0P\*\*\*

\*\*\*343632-11-1P\*\*\*

\*\*\*343632-12-2P\*\*\*

\*\*\*343632-13-3P\*\*\*

\*\*\*343632-14-4P\*\*\*

\*\*\*343632-15-5P\*\*\*

\*\*\*343632-16-6P\*\*\*

\*\*\*343632-17-7P\*\*\*

\*\*\*343632-19-9P\*\*\*

\*\*\*343632-20-2P\*\*\*

\*\*\*343632-21-3P\*\*\*

\*\*\*343969-79-9P\*\*\*

\*\*\*343969-97-1P\*\*\*

\*\*\*443118-43-2P\*\*\*

\*\*\*443118-78-3P\*\*\*

\*\*\*443760-82-5P\*\*\*

\*\*\*500736-02-7P\*\*\*

4-[[2-Methyl-1-[(1,1-dimethylethoxy)carbonyl]amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

\*\*\*500736-03-8P\*\*\*

\*\*\*500736-09-4P\*\*\*

\*\*\*500736-10-7P\*\*\*

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(A<sub>1</sub> receptor inhibitor; prepn. of pyrrolopyrimidinamines adenosine A<sub>1</sub> receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)

IT \*\*\*343632-97-3P\*\*\*

\*\*\*443760-84-7P\*\*\*

\*\*\*443760-85-8P\*\*\*

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of pyrrolopyrimidinamines adenosine A<sub>1</sub> receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)

\*\*\*\*\*

L3 ANSWER 7 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 24 Sep 2002

ACCESSION NUMBER: 2002:720128 HCAPLUS

DOCUMENT NUMBER: 137:379680

TITLE: Synthesis, Molecular Modeling Studies, and Pharmacological Activity of Selective A<sub>1</sub> Receptor Antagonists

AUTHOR(S): Bondavalli, Francesco; Botta, Maurizio; Bruno, Olga; Ciacci, Andrea; Corelli, Federico; Fossa, Paola; Lucacchini, Antonio; Manetti, Fabrizio; Martini, Claudia; Menozzi, Giulia; Mosti, Luisa; Ranise, Angelo; Schenone, Silvia; Tafi, Andrea; Trincavelli, Maria Letizia

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita degli Studi di Genova, Genoa, I-16132, Italy

SOURCE: Journal of Medicinal Chemistry (2002), 45(22), 4875-4887  
CODEN: JMCMAR; ISSN:0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We present a combined computational study aimed at identifying the three-dimensional structural properties required for different classes of compds. to show antagonistic activity toward the A<sub>1</sub> adenosine receptor (AR). Particularly, an approach combining pharmacophore mapping, mol. alignment, and pseudoreceptor generation was applied to derive a hypothesis of the interaction pathway between a set of A<sub>1</sub> AR antagonists taken from the literature and a model of the putative A<sub>1</sub> receptor. The pharmacophore model consists of seven features and represents an improvement of the N<sup>6</sup>-C<sup>8</sup> model, generally reported as the most probable pharmacophore model for A<sub>1</sub> AR agonists and antagonists. It was used to build up a pseudoreceptor model able to rationalize the relationships between structural properties and biol. data of, and external to, the training set. In fact, to further assess its statistical significance and predictive power, the pseudoreceptor was employed to predict the free energy of binding assocd. with compds. constituting a test set. While part of these mols. was also taken from the literature, the remaining compds. were designed and synthesized by our research group. All of the new compds. were tested for their affinity toward A<sub>1</sub>, A<sub>2a</sub>, and A<sub>3</sub> AR, showing interesting antagonistic activity and A<sub>1</sub> selectivity.

IT \*\*\*476006-54-9\*\*\*

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(synthesis, mol. modeling studies, and pharmacol. activity of selective A<sub>1</sub> receptor antagonists)

REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

\*\*\*\*\*

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

22

L3 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 26 Jul 2002

ACCESSION NUMBER: 2002:555495 HCAPLUS

DOCUMENT NUMBER: 137:109485

TITLE: Preparation of pyrrolopyrimidinylprolineamides and analogs as adenosine receptor antagonists

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): Osi Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 320 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

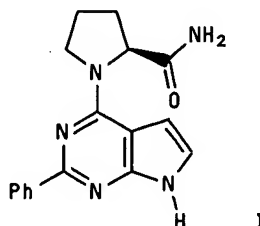
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
WO 2002057267	A1	20020725	WO 2001-US45280	20011130
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002058667	A1	20020516	US 2000-728316	20001201
US 6680322	B2	20040120		
US 2002094974	A1	20020718	US 2000-728616	20001201
US 2003036545	A1	20030220	US 2000-728607	20001201
US 6664252	B2	20031216		
EP 1347980	A1	20031001	EP 2001-997029	20011130
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
NO 2003002482	A	20030728	NO 2003-2482	20030602
PRIORITY APPLN. INFO.:				
			US 1999-169037P P	19991202
			US 2000-728316 A	20001201
			US 2000-728616 A	20001201
			US 2000-728607 A	20001204
			US 1999-168803P P	19991202
			US 1999-169036P P	19991202

L3 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2004 ACS

WO 2001-US45280 W 20011130

OTHER SOURCE(S): MARPAT 137:109485

GI



AB Title compds., e.g., I, were prepd. Data for biol. activity of title compds. were given.

IT \*\*\*251946-19-7P\*\*\*

RL: BYP (Byproduct); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrrolopyrimidinylprolineamides and analogs as adenosine receptor antagonists)

IT	***246855-41-4P***	***246855-42-5P***	***251945-90-1P***
	***251945-91-2P***	***251945-92-3P***	***251945-93-4P***
	***251945-94-5P***	***251945-95-6P***	***251945-96-7P***
	***251945-97-8P***	***251945-98-9P***	***251945-99-0P***
	***251946-00-6P***	***251946-01-7P***	***251946-06-2P***
	***251946-07-3P***	***251946-08-4P***	***251946-10-8P***
	***251946-11-9P***	***251946-12-0P***	***251946-13-1P***
	***251946-14-2P***	***251946-15-3P***	***251946-16-4P***
	***251946-17-5P***	***251946-18-6P***	***251946-20-0P***
	***251946-21-1P***	***251946-22-2P***	***251946-23-3P***
	***251946-24-4P***	***251946-25-5P***	***251946-26-6P***
	***251946-27-7P***	***251946-28-8P***	***251946-29-9P***
	***251946-30-2P***	***251946-31-3P***	***251946-32-4P***
	***251946-33-5P***	***251946-34-6P***	***251946-35-7P***
	***251946-36-8P***	***251946-37-9P***	***251946-38-0P***
	***251946-39-1P***	***251946-40-4P***	***251946-41-5P***
	***251946-42-6P***	***251946-43-7P***	***251946-44-8P***
	***251946-45-9P***	***251946-46-0P***	***251946-47-1P***
	***251946-48-2P***	***251946-49-3P***	***251946-50-6P***
	***251946-52-8P***	***251946-54-0P***	***251946-55-1P***
	***251946-56-2P***	***251946-57-3P***	***251946-58-4P***
	***251946-59-5P***	***251947-22-5P***	***251947-24-7P***

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE 24

L3 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2004 ACS

***343632-03-1P***	***343632-05-3P***	***343632-06-4P***
***343632-07-5P***	***343632-08-6P***	***343632-09-7P***
***343632-10-0P***	***343632-11-1P***	***343632-12-2P***
***343632-13-3P***	***343632-14-4P***	***343632-16-6P***
***343632-17-7P***	***343632-19-9P***	***343632-20-2P***
***343632-21-3P***	***343632-31-5P***	***343632-35-9P***
***343632-37-1P***	***343632-38-2P***	***343632-50-8P***
***343969-79-9P***	***343969-97-1P***	***443118-47-6P***
***443760-78-9P***	***443760-79-0P***	***443760-80-3P***
***443760-82-5P***		

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrrolopyrimidinylprolineamides and analogs as adenosine receptor antagonists)

IT \*\*\*443760-84-7P\*\*\* \*\*\*443760-85-8P\*\*\*

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of pyrrolopyrimidinylprolineamides and analogs as adenosine receptor antagonists)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

\*\*\*\*\*

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

25

L3 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 19 Jul 2002

ACCESSION NUMBER: 2002:540257 HCAPLUS

DOCUMENT NUMBER: 137:109288

TITLE: Preparation of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A<sub>3</sub> receptor

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 83 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

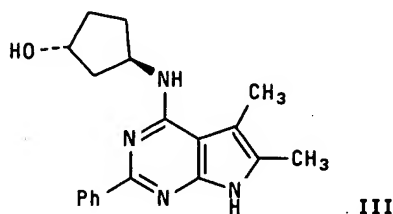
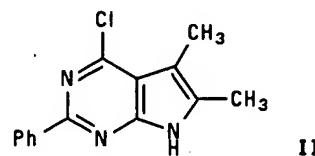
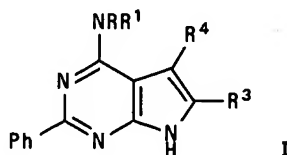
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002094974	A1	20020718	US 2000-728616	20001201
WO 2002057267	A1	20020725	WO 2001-US45280	20011130
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1347980	A1	20031001	EP 2001-997029	20011130
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
NO 2003002482	A	20030728	NO 2003-2482	20030602
PRIORITY APPLN. INFO.:				
			US 1999-169036P P	19991202
			US 1999-169037P P	19991202
			US 2000-728316 A	20001201
			US 2000-728616 A	20001201
			US 2000-728607 A	20001204
			WO 2001-US45280 W	20011130

OTHER SOURCE(S): MARPAT 137:109288

GI



L3 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2004 ACS



**AB** Pyrrolopyrimidines **I** [ $R = 3\text{-hydroxycyclopentylamino ethylamino carbonylamino Pr, N,N-diethylamino carbonylamino Et, thioacetamido Et, 3-amino acetyloxy cyclopentyl, 3-hydroxycyclopentyl, 2-pyrrolyl carbonyl aminoethyl, 2-imidazolinone Et, 1-aminocarbonyl-2-methylpropyl, 1-aminocarbonyl-2-Ph Et, 3-hydroxyazetidino, 2-imidazoleethyl, acetamidoethyl, 1-(*R*)-phenyl-2-hydroxyethyl, N-methylaminocarbonyl pyridyl-2-methyl;  $R^1 = H$ ;  $RR^1N = 3\text{-hydroxypyrrolidino, 3-methyloxy carbonylmethyl pyrrolidino, 3-aminocarbonylmethyl pyrrolidino, 3-hydroxymethyl piperidino}$ ;  $R^3, R^4 = H, (\text{un})\text{substituted alkyl, aryl}$ ] are prep'd. as selective inhibitors of adenosine receptors, particularly the adenosine  $A_3$  receptor, for the treatment of diseases such as asthma, diarrhea, chronic obstructive pulmonary disease, allergic rhinitis, or for the treatment of eye damage caused either by disease or injury. Human adenosine receptors are transformed into yeast; the modified yeast are used to assay the invention compds. **I** for their adenosine receptor binding and selectivities. E.g., 1-(1-phenylethyl)-2-amino-3-cyano-4,5-dimethylpyrrole is acylated with  $\text{PhCOCl}$  to give the benzamide which undergoes cyclocondensation with concd.  $\text{H}_2\text{SO}_4$  in MeOH to give a pyrrolopyrimidinone; removal of the phenethyl group with polyphosphoric acid and chlorination of the pyrrolopyrimidinone with  $\text{POCl}_3$  gives the intermediate chloropyrrolopyrimidine **II**. E.g., addn. of amines such as trans-3-amino-1-cyclopentanol to **II** in DMSO gives aminopyrrolopyrimidines such as **III**. **III** has a  $K_i$  for the adenosine  $A_1$  receptor of 29 nM and a  $K_i$  for the adenosine  $A_3$  receptor of 3.1 nM while binding to the adenosine  $A_{2a}$  and  $A_{2b}$  receptors with  $K_i$  values of 191 nM and 1143 nM, resp. Formulations of these compds. are claimed (no data). Methods for the prep'n. of **I** from the acylation of aminopyrroles with acyl chlorides followed by cyclocondensation and deprotection, chlorination, and substitution of the chlorine atom with an amine are claimed.$

**IT** \*\*\*251946-42-6P\*\*\*      \*\*\*443118-78-3P\*\*\*

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL

## L3 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2004 ACS

(Biological study); PREP (Preparation); USES (Uses)

(intermediate; prepn. of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A<sub>3</sub> receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from injuries or disease)

## IT \*\*\*343632-97-3P\*\*\*

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A<sub>3</sub> receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from injuries or disease)

IT ***177499-41-1P***	***246855-41-4P***	***246855-42-5P***
***246855-44-7P***	***246855-45-8P***	***246855-46-9P***
***246855-48-1P***	***251945-90-1P***	***251945-91-2P***
***251945-92-3P***	***251945-93-4P***	***251945-94-5P***
***251945-95-6P***	***251945-96-7P***	***251945-97-8P***
***251945-98-9P***	***251946-03-9P***	***251946-06-2P***
***251946-07-3P***	***251946-08-4P***	***251946-10-8P***
***251946-11-9P***	***251946-12-0P***	***251946-13-1P***
***251946-14-2P***	***251946-15-3P***	***251946-16-4P***
***251946-17-5P***	***251946-18-6P***	***251946-19-7P***
***251946-20-0P***	***251946-21-1P***	***251946-22-2P***
***251946-23-3P***	***251946-24-4P***	***251946-25-5P***
***251946-26-6P***	***251946-27-7P***	***251946-28-8P***
***251946-29-9P***	***251946-30-2P***	***251946-31-3P***
***251946-32-4P***	***251946-33-5P***	***251946-34-6P***
***251946-35-7P***	***251946-36-8P***	***251946-37-9P***
***251946-38-0P***	***251946-39-1P***	***251946-40-4P***
***251946-41-5P***	***251946-44-8P***	***251946-45-9P***
***251946-46-0P***	***251946-47-1P***	***251946-48-2P***
***251946-49-3P***	***251946-50-6P***	***251946-52-8P***
***251946-57-3P***	***251946-58-4P***	***251946-59-5P***
***251947-22-5P***	***251947-24-7P***	***343632-04-2P***
***343632-06-4P***	***343632-11-1P***	***343632-13-3P***
***343632-14-4P***	***343632-15-5P***	***343632-17-7P***
***343632-31-5P***	***343632-32-6P***	***343632-33-7P***
***343632-35-9P***	***343632-36-0P***	***343632-37-1P***
***343632-38-2P***	***343632-50-8P***	***343632-77-9P***
***343632-78-0P***	***343632-79-1P***	***343633-16-9P***
***343969-97-1P***	***443118-21-6P***	***443118-22-7P***
***443118-23-8P***	***443118-24-9P***	***443118-26-1P***

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE 28

L3 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2004 ACS

***443118-36-3P***	***443118-41-0P***	***443118-42-1P***
***443118-43-2P***	***443118-44-3P***	***443118-45-4P***
***443118-46-5P***	***443118-47-6P***	***443118-48-7P***
***443118-49-8P***	***443118-50-1P***	***443118-51-2P***
***443118-52-3P***	***443118-53-4P***	***443118-54-5P***
***443118-55-6P***	***443118-56-7P***	***443118-57-8P***
***443118-58-9P***	***443118-59-0P***	***443118-60-3P***
***443118-61-4P***	***443118-62-5P***	***443118-63-6P***
***443118-64-7P***	***443118-65-8P***	***443118-66-9P***
***443118-67-0P***	***443118-68-1P***	***443118-69-2P***
***443118-70-5P***	***443118-71-6P***	***443118-72-7P***
***443118-73-8P***		

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(invention compd.; prepn. of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A<sub>3</sub> receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from injuries or disease)

\*\*\*\*\*

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

29

L3 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 18 May 2002

ACCESSION NUMBER: 2002:368992 HCAPLUS

DOCUMENT NUMBER: 136:386128

TITLE: Synthesis and use of substituted pyrrolo[2,3-b]pyrimidines as selective adenosine A<sub>1</sub>, A<sub>2a</sub> and A<sub>3</sub> receptor antagonists

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 79 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002058667	A1	20020516	US 2000-728316	20001201
US 6680322	B2	20040120		
WO 2002057267	A1	20020725	WO 2001-US45280	20011130

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1347980 A1 20031001 EP 2001-997029 20011130

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

NO 2003002482 A 20030728 NO 2003-2482 20030602

PRIORITY APPLN. INFO.:

US 1999-168803P P 19991202

US 1999-169037P P 19991202

US 2000-728316 A 20001201

US 2000-728616 A 20001201

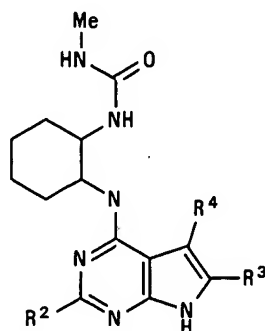
US 2000-728607 A 20001204

WO 2001-US45280 W 20011130

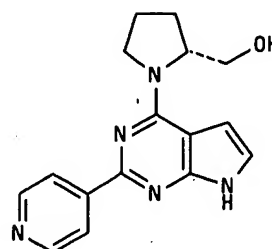
OTHER SOURCE(S): MARPAT 136:386128

GI

L3 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2004 ACS



I



II

AB Title compds. I and analogs [ $R^2$  = 5-6 membered arom. ring;  $R^{3-4}$  = H, alkyl] were prepd. Over 100 examples were provided. Intermediate 4-chloro-7H-pyrrolo[2,3-d]pyrimidines were prepd. by several routes from appropriately substituted cyano-pyrroles. Thus, 4-chloro-2-(4-pyridyl)-7H-pyrrolo[2,3-d]pyrimidine hydrochloride was reacted with D-prolinol (2.3 mol equiv) in DMSO at 120°C for 18 h to yield II in 13% yield after purifn. Compd. I [ $R^2$  = Ph;  $R^{3-4}$  = Me] exhibited 10-fold selectivity for binding to the adenosine  $A_1$  receptor than to  $A_{2a}$ ,  $A_{2b}$  or  $A_3$  receptors. ClogP values were detd. for selected example compds. I are useful for the treatment of COPD, allergic rhinitis, etc.

IT \*\*\*251946-19-7P\*\*\*, 1H-Pyrrolo[2,3-d]pyrimidin-4-amine,  
N-3-cyclohexen-1-yl-5,6-dimethyl-2-phenyl-

RL: BSU (Biological study, unclassified); BYP (Byproduct); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine  $A_1$ ,  $A_{2a}$  and  $A_3$  receptor antagonists)

IT \*\*\*251946-18-6P\*\*\*, Cyclohexanol,

4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-benzoate (ester), *cis*-

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine  $A_1$ ,  $A_{2a}$  and  $A_3$  receptor antagonists)

IT \*\*\*246855-41-4P\*\*\*, Cyclohexanol,

4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-*trans* \*\*\*246855-42-

5P\*\*\*, Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-

\*\*\*251945-90-1P\*\*\*, Cyclohexanol,

4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, *trans*- \*\*\*251945-91-

L3 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2004 ACS

2P\*\*\* , Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*-  
 \*\*\*251945-92-3P\*\*\* , Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*-  
 \*\*\*251945-93-4P\*\*\* , Cyclohexanol,  
 4-[[5,6-dimethyl-2-(3-pyridinyl)-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
 \*\*\*251945-94-5P\*\*\* , Cyclohexanol,  
 4-[[2-(2-furanyl)-5,6-dimethyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
 \*\*\*251945-95-6P\*\*\* , Cyclohexanol,  
 4-[[2-(3-furanyl)-5,6-dimethyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
 \*\*\*251945-96-7P\*\*\* , Cyclohexanol,  
 4-[(2-cyclopentyl-5,6-dimethyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*-  
 \*\*\*251945-97-8P\*\*\* , Cyclohexanol,  
 4-[[5,6-dimethyl-2-(2-thienyl)-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
 \*\*\*251945-98-9P\*\*\* , Cyclohexanol,  
 4-[[5,6-dimethyl-2-(3-thienyl)-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
 \*\*\*251945-99-0P\*\*\* , Cyclohexanol,  
 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
 \*\*\*251946-00-6P\*\*\* , Cyclohexanol,  
 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
 \*\*\*251946-01-7P\*\*\* , Cyclohexanol,  
 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-  
 \*\*\*251946-03-9P\*\*\* , Cyclohexanol,  
 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*  
 \*\*\*251946-04-0P\*\*\* , 1,2-Cyclohexanediol,  
 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*  
 \*\*\*251946-05-1P\*\*\* , 1,2-Cyclohexanediol,  
 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*S*)-*rel*  
 \*\*\*251946-06-2P\*\*\* , Cyclopentanol,  
 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*  
 \*\*\*251946-07-3P\*\*\* , Cyclopentanol,  
 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,3*R*)-*rel*  
 \*\*\*251946-08-4P\*\*\* , Cyclopentanol,  
 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,3*S*)-*rel*  
 \*\*\*251946-09-5P\*\*\* , Propanamide,  
 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, \*\*\*251946-11-9P\*\*\*,  
 Propanamide, *N*-(cyclopropylmethyl)-3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-  
 \*\*\*251946-12-0P\*\*\* , Acetamide,  
 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, \*\*\*251946-13-1P\*\*\*, Acetamide,  
 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-*N*-methyl-  
 \*\*\*251946-14-2P\*\*\* ,  $\beta$ -Alanine, *N*-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidin-4-yl)-,  
 1,1-dimethylethyl ester \*\*\*251946-15-3P\*\*\* , Ethanol,

L3 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2004 ACS

2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- \*\*\*251946-16-4P\*\*\*, 1-Propanol,  
3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- \*\*\*251946-17-5P\*\*\*, 1-Butanol,  
4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- \*\*\*251946-20-0P\*\*\*,  
Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *cis*  
\*\*\*251946-21-1P\*\*\*, Propanamide,  
3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-*N,N*-dimethyl-  
\*\*\*251946-22-2P\*\*\*, Formamide,  
*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- \*\*\*251946-  
23-3P\*\*\*, Acetamide,  
*N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-  
\*\*\*251946-24-4P\*\*\*,  $\beta$ -Alanine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)-  
\*\*\*251946-25-5P\*\*\*, 1,3-Propanediamine,  
*N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)- \*\*\*251946-26-6P\*\*\*, Propanamide,  
3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-*N*-methyl-  
\*\*\*251946-27-7P\*\*\*, Cyclopropanecarboxamide,  
*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- \*\*\*251946-  
28-8P\*\*\*, Propanamide,  
*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2-methyl-,  
\*\*\*251946-29-9P\*\*\*, Propanamide,  
*N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-  
\*\*\*251946-30-2P\*\*\*, Methanesulfonamide,  
*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- \*\*\*251946-  
31-3P\*\*\*, 1,2-Ethanediamine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)-  
\*\*\*251946-32-4P\*\*\*, Propanamide,  
*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- \*\*\*251946-  
33-5P\*\*\*, Urea,  
*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-*N'*-methyl-  
\*\*\*251946-34-6P\*\*\*, Urea,  
*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-*N'*-ethyl-  
\*\*\*251946-35-7P\*\*\*, Propanamide,  
*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2-oxo-  
\*\*\*251946-36-8P\*\*\*, Urea,  
[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- \*\*\*251946-37-  
9P\*\*\*, Acetamide,  
*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-  
\*\*\*251946-38-0P\*\*\*, Acetamide,  
*N*-[(1*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-  
\*\*\*251946-39-1P\*\*\*, Acetamide,  
*N*-[(2*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-  
\*\*\*251946-40-4P\*\*\*, Acetamide,

L3 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2004 ACS

*N*-[(1*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-  
 \*\*\*251946-41-5P\*\*\* , Acetamide,

*N*-[(2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-  
 \*\*\*251946-42-6P\*\*\* , Carbamic acid,

[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-, 1,1-dimethylethyl ester  
 \*\*\*251946-43-7P\*\*\* , Carbamic acid,

[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-, 1,1-dimethylethyl  
 ester \*\*\*251946-44-8P\*\*\* , Acetamide,

*N*-[(1*S*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-  
 \*\*\*251946-45-9P\*\*\* , Acetamide,

*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1,1-dimethylethyl]-  
 \*\*\*251946-46-0P\*\*\* , Acetamide,

*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-  
 \*\*\*251946-47-1P\*\*\* , Acetamide,

*N*-[(1*R*,2*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-  
 \*\*\*251946-48-2P\*\*\* , Ethanol,

2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, acetate (ester)  
 \*\*\*251946-49-3P\*\*\* , Propanamide,

3-amino-*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-  
 \*\*\*251946-50-6P\*\*\* , Butanoic acid,

4-[[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]amino]-4-oxo-  
 \*\*\*251946-52-8P\*\*\* , Glycine,

(1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*-,  
 mono(trifluoroacetate) \*\*\*251946-54-0P\*\*\* , Urea,

*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-*N*'-methyl-  
 \*\*\*251946-55-1P\*\*\* , Acetamide,

*N*-[1-[[[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]methyl]propyl]-  
 \*\*\*251946-56-2P\*\*\* , Urea,

*N*-[1-[[[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]methyl]propyl]-*N*'-methyl-  
 \*\*\*251946-57-3P\*\*\* , Cyclohexanol,

4-[[2-(3-chlorophenyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- \*\*\*251946-58-  
 4P\*\*\* , Cyclohexanol, 4-[[2-(3-fluorophenyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-

\*\*\*251946-59-5P\*\*\* , Cyclohexanol,

4-[[2-(4-pyridinyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- \*\*\*251947-22-  
 5P\*\*\* , Acetamide,

*N*-[*trans*-4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-  
 \*\*\*251947-24-7P\*\*\* , Methanesulfonamide,

*N*-[*trans*-4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-  
 \*\*\*343631-95-8P\*\*\* , Propanamide,

*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2,2-dimethyl-



L3 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2004 ACS

\*\*\*343631-96-9P\*\*\* , 1,2-Cyclohexanediamine,  
N-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (1R,2R)- \*\*\*343631-97-  
0P\*\*\* , Propanamide,  
3-[[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]amino]-  
\*\*\*343631-99-2P\*\*\* , Acetamide,  
2-(cyclopropylamino)-N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-  
\*\*\*343632-03-1P\*\*\* , 1,2-Cyclohexanediol,  
4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4R)-rel  
\*\*\*343632-04-2P\*\*\* , Cyclohexanol,  
4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, benzoate (ester)  
\*\*\*343632-05-3P\*\*\* , Cyclohexanol,  
4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans-  
\*\*\*343632-06-4P\*\*\* , Cyclohexanol,  
4-[[2-(3-furanyl)-5,6-dimethyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans-  
\*\*\*343632-07-5P\*\*\* , Cyclohexanol,  
4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans-  
\*\*\*343632-08-6P\*\*\* , 7H-Pyrrolo[2,3-d]pyrimidin-4-amine,  
5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-N-(3-pyridinylmethyl)- \*\*\*343632-09-7P\*\*\* ,  
Acetamide,  
N-[2-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]-  
\*\*\*343632-10-0P\*\*\* , 7H-Pyrrolo[2,3-d]pyrimidin-4-amine,  
5,6-dimethyl-N-(2-methylpropyl)-2-phenyl-7-(1-phenylethyl)- \*\*\*343632-11-1P\*\*\* , Propanamide,  
N-[3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]-2-methyl-  
\*\*\*343632-12-2P\*\*\* , Urea,  
N-[3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]-N'-methyl-  
\*\*\*343632-13-3P\*\*\* , Acetamide,  
N-[4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]butyl]- \*\*\*343632-  
14-4P\*\*\* , Urea,  
N-[4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]butyl]-N'-methyl-  
\*\*\*343632-15-5P\*\*\* , Cyclopropanecarboxamide,  
1-amino-N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-  
\*\*\*343632-16-6P\*\*\* , Propanamide,  
3-amino-N-[3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]-  
\*\*\*343632-17-7P\*\*\* , Acetamide,  
2-amino-N-[3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]-  
\*\*\*343632-19-9P\*\*\* , Urea,  
N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]cyclohexyl]-N'-methyl-  
\*\*\*343632-20-2P\*\*\* , Acetamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-  
\*\*\*343632-21-3P\*\*\* , Urea,  
N-[2-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]-N'-methyl-

L3 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2004 ACS

\*\*\*343632-69-9P\*\*\* , 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-phenyl-*N*-[2-(1*H*-pyrrol-2-yl)ethyl]-  
 \*\*\*343632-70-2P\*\*\* , Urea,  
*N*-[(2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-  
 \*\*\*343632-71-3P\*\*\* , Urea,  
*N*-[(1*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-  
 \*\*\*343632-72-4P\*\*\* , Urea,  
*N*-[(1*R*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-  
 \*\*\*343632-73-5P\*\*\* , Urea,  
*N*-[(1*S*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-  
 \*\*\*343632-77-9P\*\*\* , Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*S*,3*R*)-  
 \*\*\*343632-78-0P\*\*\* , Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-,  
 (1*R*,3*S*)- \*\*\*343632-79-1P\*\*\* , Cyclopentanol,  
 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (3*S*)- \*\*\*343633-16-9P\*\*\* ,  
 Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*S*,3*S*)-  
 \*\*\*343969-79-9P\*\*\* , 1,2-Cyclohexanediol,  
 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*S*,4*S*)-*rel*  
 \*\*\*343969-97-1P\*\*\* , 1,2-Cyclopentenediol,  
 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1 $\alpha$ ,2 $\alpha$ ,4 $\beta$ )

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and use of substituted 7*H*-pyrrolo[2,3-*b*]pyrimidines as selective adenosine A<sub>1</sub>, A<sub>2a</sub> and A<sub>3</sub> receptor antagonists)

IT \*\*\*343632-96-2P\*\*\* , Carbamic acid,  
 [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-, 1,1-dimethylethyl ester  
 \*\*\*343632-97-3P\*\*\* , Glycine, *N*-[(1,1-dimethylethoxy)carbonyl]-,  
 (1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*-  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and use of substituted 7*H*-pyrrolo[2,3-*b*]pyrimidines as selective adenosine A<sub>1</sub>, A<sub>2a</sub> and A<sub>3</sub> receptor antagonists)

\*\*\*\*\*

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

36

L3 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 08 Jun 2001

ACCESSION NUMBER: 2001:416773 HCAPLUS

DOCUMENT NUMBER: 135:46190

TITLE: Synthesis and use of substituted pyrrolo[2,3-b]pyrimidines as selective adenosine A<sub>1</sub>, A<sub>2a</sub> and A<sub>3</sub> receptor antagonists

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): Osi Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 368 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

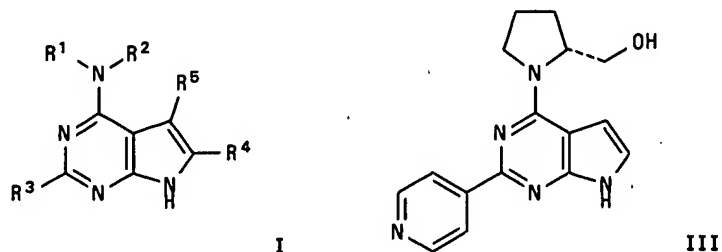
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WD 2001039777	A1	20010607	WD 2000-US32702	20001201
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6686366	B1	20040203	US 1999-454075	19991202
EP 1246623	A1	20021009	EP 2000-988011	20001201
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003519102	T2	20030617	JP 2001-541509	20001201
PRIORITY APPLN. INFO.:				
			US 1999-454074 A	19991202
			US 1999-454075 A	19991202
			US 1999-454254 A	19991202
			US 1998-87702P P	19980602
			US 1999-123216P P	19990308
			US 1999-126527P P	19990326
			WO 1999-US12135 A2	19990601
			WO 2000-US32702 W	20001201

OTHER SOURCE(S): MARPAT 135:46190

L3 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2004 ACS  
GI



AB The synthesis of compds. I, their binding to adenosine receptors and use are described [wherein; R<sup>1</sup>, R<sup>2</sup> = H, (un)substituted alkyl or NR<sup>1</sup>R<sup>2</sup> = (un)substituted 4-8 membered ring; R<sup>3</sup> = (un)substituted 4-6 membered (arom.) ring; R<sup>4</sup>, R<sup>5</sup> = H, (un)substituted alkyl, aryl (with some exceptions)]. Over 100 examples are provided. Intermediate 4-chloro-7H-pyrrolo[2,3-d]pyrimidines were prepd. by several routes from appropriately substituted cyano-pyrroles. Thus, 4-chloro-2-(4-pyridyl)-7H-pyrrolo[2,3-d]pyrimidine hydrochloride was reacted with D-prolinol (2.3 mol equiv) in DMSO at 120°C for 18 h to yield III in 13% yield after purifn. Compd. I [R<sup>1</sup> = AcNHCH<sub>2</sub>CH<sub>2</sub>; R<sup>2</sup> = H; R<sup>3</sup> = Ph; R<sup>4</sup>, R<sup>5</sup> = Me; II] exhibited selective binding to adenosine receptor A<sub>1</sub> with IC<sub>50</sub> = 82.8 nM. Compd. II also had K<sub>i</sub> = 9.8 nM (vs. K<sub>i</sub> = 7.1 for control ligand 8-cyclopentyl-1,3-dipropylxanthine (DPCPX)). Pyrimidine III binds 5 times more selectively to adenosine receptor A<sub>2a</sub> than A<sub>1</sub>, A<sub>2b</sub> or A<sub>3</sub> (no data). Compd. I [R<sup>1</sup> = AcNH(CH<sub>2</sub>)<sub>4</sub>; R<sup>2</sup> = H; R<sup>3</sup> = Ph; R<sup>4</sup>, R<sup>5</sup> = Me] is 10 times more selective for A<sub>3</sub> than the other receptor subtypes. ClogP (calcd. partition coeff. between octanol and H<sub>2</sub>O) values were detd. for selected example compds. Claimed uses of I includes administration of a systemic formulation (i.e. ophthalmic) for the treatment of a disease assocd. with A<sub>1</sub>, A<sub>2a</sub>, and A<sub>3</sub> adenosine receptors in a subject.

IT \*\*\*251946-19-7P\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BYP (Byproduct); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A<sub>1</sub>, A<sub>2a</sub> and A<sub>3</sub> receptor antagonists)

IT \*\*\*251946-18-6P\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A<sub>1</sub>, A<sub>2a</sub> and A<sub>3</sub> receptor antagonists)

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

38

L3 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2004 ACS

IT	***246855-41-4P***	***246855-42-5P***	***251945-90-1P***
	***251945-91-2P***	***251945-92-3P***	***251945-93-4P***
	***251945-94-5P***	***251945-95-6P***	***251945-96-7P***
	***251945-97-8P***	***251945-98-9P***	***251945-99-0P***
	***251946-00-6P***	***251946-01-7P***	***251946-03-9P***
	***251946-04-0P***	***251946-05-1P***	***251946-06-2P***
	***251946-07-3P***	***251946-08-4P***	***251946-09-5P***
	***251946-10-8P***	***251946-11-9P***	***251946-12-0P***
	***251946-13-1P***	***251946-14-2P***	***251946-15-3P***
	***251946-16-4P***	***251946-17-5P***	***251946-20-0P***
	***251946-21-1P***	***251946-22-2P***	***251946-23-3P***
	***251946-24-4P***	***251946-25-5P***	***251946-26-6P***
	***251946-27-7P***	***251946-28-8P***	***251946-29-9P***
	***251946-30-2P***	***251946-31-3P***	***251946-32-4P***
	***251946-33-5P***	***251946-34-6P***	***251946-35-7P***
	***251946-36-8P***	***251946-37-9P***	***251946-38-0P***
	***251946-39-1P***	***251946-40-4P***	***251946-41-5P***
	***251946-42-6P***	***251946-43-7P***	***251946-44-8P***
	***251946-45-9P***	***251946-46-0P***	***251946-47-1P***
	***251946-48-2P***	***251946-49-3P***	***251946-50-6P***
	***251946-52-8P***	***251946-54-0P***	***251946-55-1P***
	***251946-56-2P***	***251946-57-3P***	***251946-58-4P***
	***251946-59-5P***	***251947-22-5P***	***251947-24-7P***
	***343631-95-8P***	***343631-96-9P***	***343631-97-0P***
	***343631-99-2P***	***343632-03-1P***	***343632-04-2P***
	***343632-05-3P***	***343632-06-4P***	***343632-07-5P***
	***343632-08-6P***	***343632-09-7P***	***343632-10-0P***
	***343632-11-1P***	***343632-12-2P***	***343632-13-3P***
	***343632-14-4P***	***343632-15-5P***	***343632-16-6P***
	***343632-17-7P***	***343632-19-9P***	***343632-20-2P***
	***343632-21-3P***	***343632-31-5P***	***343632-32-6P***
	***343632-33-7P***	***343632-35-9P***	***343632-36-0P***
	***343632-37-1P***	***343632-38-2P***	***343632-50-8P***
	***343632-69-9P***	***343632-70-2P***	***343632-71-3P***
	***343632-72-4P***	***343632-73-5P***	***343632-77-9P***
	***343632-78-0P***	***343632-79-1P***	***343633-16-9P***
	***343969-79-9P***	***343969-97-1P***	

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

L3 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2004 ACS

(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A<sub>1</sub>, A<sub>2a</sub> and A<sub>3</sub> receptor antagonists)

IT \*\*\*343632-96-2P\*\*\* \*\*\*343632-97-3P\*\*\*

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A<sub>1</sub>, A<sub>2a</sub> and A<sub>3</sub> receptor antagonists)

REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

\*\*\*\*\*

L3 ANSWER 12 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 14 Nov 2000

ACCESSION NUMBER: 2000:792835 HCAPLUS

DOCUMENT NUMBER: 134:100695

TITLE: 7-Deazaadenines Bearing Polar Substituents: Structure-Activity Relationships of New A<sub>1</sub> and A<sub>3</sub> Adenosine Receptor Antagonists

AUTHOR(S): Hess, Sonja; Mueller, Christa E.; Frobenius, Wolfram; Reith, Ulrike; Klotz, Karl-Norbert; Eger, Kurt

CORPORATE SOURCE: Pharmaceutical Chemistry Institute of Pharmacy, University of Leipzig, Leipzig, D-04103, Germany

SOURCE: Journal of Medicinal Chemistry (2000), 43(24), 4636-4646  
CODEN: JMCMAR; ISSN:0022-2623

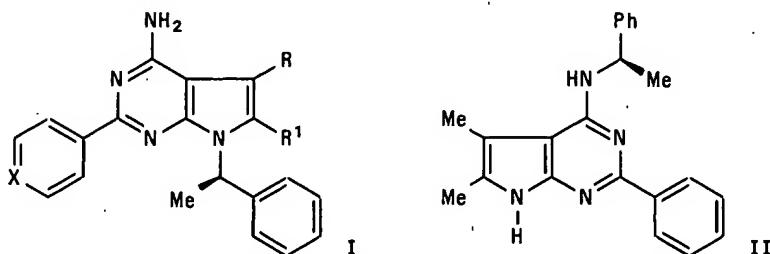
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:100695

GI



**AB** A series of 28 new pyrrolo[2,3-d]pyrimidine-4-amines, pyrimido[4,5-b]indole-4-amines, and tetrahydropyrimido[4,5-b]indole-4-amines was synthesized and their adenosine receptor affinity detd. in radioligand binding assays at rat A<sub>1</sub> and A<sub>2A</sub> adenosine receptors (ARs). Selected compds. were addnl. investigated in binding assays at recombinant A<sub>3</sub> ARs. The 2-Ph residue in (R)-7-(1-methylbenzyl)-2-phenylpyrrolo[2,3-d]pyrimidine-4-amine (ADPEP) I (R = R<sup>1</sup> = Me, X = CH) and in the corresponding pyrimido[4,5-b]indole (APEPI) I (RR<sup>1</sup> = CH:CHCH:CH, X = CH) could be bioisosterically replaced by heterocyclic rings, such as 2-thienyl and 4-pyridyl. The resulting compds. retained high affinity and selectivity for A<sub>1</sub> ARs. Judging from the investigation of selected compds., it appears that they are also potent at human A<sub>1</sub> ARs and selective not only vs. A<sub>2A</sub> ARs but also highly selective vs. A<sub>2B</sub> and A<sub>3</sub> ARs. The p-pyridyl-substituted derivs. I (R = R<sup>1</sup> = Me, X = N) and (APPPPI) I (RR<sup>1</sup> = CH:CHCH:CH, X = X) may be interesting pharmacol. tools due to their fluorescent properties. Pyrrolo[2,3-d]pyrimidine-4-amine derivs. which were simultaneously substituted at N7 and N4, combining the substitution pattern of ADPEP and DPEAP (II), showed very low affinity for

## L3 ANSWER 12 OF 30 HCAPLUS COPYRIGHT 2004 ACS

A<sub>1</sub> ARs. This finding supports previously published hypothesis of different binding modes for pyrrolopyrimidines, such as ADPEP and DPEAP. DPEAP was found to exhibit high affinity for human A<sub>3</sub> ARs (K<sub>i</sub> = 28 nM), whereas N<sup>4</sup>-unsubstituted analogs were inactive. DPEAP and related compds. provide new leads for the development of antagonists for the human A<sub>3</sub> AR.

IT \*\*\*130147-80-7\*\*\* \*\*\*177499-40-0\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(prepn. of 7-deazaadenines bearing polar substituents and their structure-activity relationships as A<sub>1</sub> and A<sub>3</sub> adenosine receptor antagonists)

IT \*\*\*319481-19-1P\*\*\* \*\*\*319481-20-4P\*\*\* \*\*\*319481-21-5P\*\*\*

\*\*\*319481-22-6P\*\*\* \*\*\*319481-23-7P\*\*\* \*\*\*319481-24-8P\*\*\*

\*\*\*319481-25-9P\*\*\* \*\*\*319481-26-0P\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 7-deazaadenines bearing polar substituents and their structure-activity relationships as A<sub>1</sub> and A<sub>3</sub> adenosine receptor antagonists)

IT \*\*\*319481-39-5P\*\*\* \*\*\*319481-41-9P\*\*\* \*\*\*319481-47-5P\*\*\*

\*\*\*319481-48-6P\*\*\* \*\*\*319481-49-7P\*\*\* \*\*\*319481-50-0P\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of 7-deazaadenines bearing polar substituents and their structure-activity relationships as A<sub>1</sub> and A<sub>3</sub> adenosine receptor antagonists)

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

\*\*\*\*\*



# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE 42

L3 ANSWER 13 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 10 Dec 1999

ACCESSION NUMBER: 1999:783937 HCAPLUS

DOCUMENT NUMBER: 132:22973

TITLE: Preparation of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): Cadus Pharmaceutical Corp., USA

SOURCE: PCT Int. Appl., 169 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

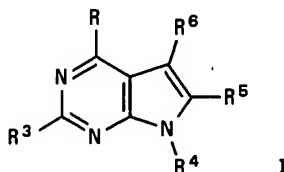
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
WO 9962518	A1	19991209	WO 1999-US12135	19990601
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2334200	AA	19991209	CA 1999-2334200	19990601
AU 9942265	A1	19991220	AU 1999-42265	19990601
AU 763658	B2	20030731		
BR 9911612	A	20010206	BR 1999-11612	19990601
EP 1082120	A1	20010314	EP 1999-926107	19990601
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002516861	T2	20020611	JP 2000-551774	19990601
US 6686366	B1	20040203	US 1999-454075	19991202
NO 2000006090	A	20010131	NO 2000-6090	20001130
US 2002028782	A1	20020307	US 2000-728229	20001201
PRIORITY APPLN. INFO.:				
			US 1998-87702P P	19980602
			US 1999-123216P P	19990308
			US 1999-126527P P	19990326
			WO 1999-US12135 W	19990601
OTHER SOURCE(S): MARPAT 132:22973				

L3 ANSWER 13 OF 30 HCAPLUS COPYRIGHT 2004 ACS  
GI



AB Title compds. [I; R = NR<sup>1</sup>R<sup>2</sup>; R<sup>1</sup>-R<sup>4</sup> = H, alkyl, aryl, etc.; NR<sup>1</sup>R<sup>2</sup> = heterocyclyl; R<sup>5</sup>,R<sup>6</sup> = H, halo, alkyl, aryl, etc.; R<sup>4</sup>R<sup>5</sup>,R<sup>5</sup>R<sup>6</sup> = atoms to complete a ring] were prepd. Thus, 2-amino-3-cyano-4,5-dimethyl-1-(1-phenylethyl)pyrrole was N-benzoylated and the product cyclized to give, after deprotection and chlorination, I (R<sup>3</sup> = Ph, R<sup>4</sup> = H, R<sup>5</sup> = R<sup>6</sup> = Me)(II; R = Cl) which was aminated by trans-4-hydroxycyclohexylamine to give II (R = trans-4-hydroxycyclohexylamino). Data for biol. activity of I were given.

IT	***246855-41-4P***	***246855-42-5P***	***251945-90-1P***
	***251945-91-2P***	***251945-92-3P***	***251945-93-4P***
	***251945-94-5P***	***251945-95-6P***	***251945-96-7P***
	***251945-97-8P***	***251945-98-9P***	***251945-99-0P***
	***251946-00-6P***	***251946-01-7P***	***251946-03-9P***
	***251946-04-0P***	***251946-05-1P***	***251946-06-2P***
	***251946-07-3P***	***251946-08-4P***	***251946-09-5P***
	***251946-10-8P***	***251946-11-9P***	***251946-12-0P***
	***251946-13-1P***	***251946-14-2P***	***251946-15-3P***
	***251946-16-4P***	***251946-17-5P***	***251946-18-6P***
	***251946-19-7P***	***251946-20-0P***	***251946-21-1P***
	***251946-22-2P***	***251946-23-3P***	***251946-24-4P***
	***251946-25-5P***	***251946-26-6P***	***251946-27-7P***
	***251946-28-8P***	***251946-29-9P***	***251946-30-2P***
	***251946-31-3P***	***251946-32-4P***	***251946-33-5P***
	***251946-34-6P***	***251946-35-7P***	***251946-36-8P***
	***251946-37-9P***	***251946-38-0P***	***251946-39-1P***
	***251946-40-4P***	***251946-41-5P***	***251946-42-6P***
	***251946-43-7P***	***251946-44-8P***	***251946-45-9P***
	***251946-46-0P***	***251946-47-1P***	***251946-48-2P***
	***251946-49-3P***	***251946-50-6P***	***251946-52-8P***
	***251946-54-0P***	***251946-55-1P***	***251946-56-2P***
	***251946-57-3P***	***251946-58-4P***	***251946-59-5P***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified);

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

44

L3 ANSWER 13 OF 30 HCAPLUS COPYRIGHT 2004 ACS

SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation);  
USES (Uses)

(prepn. of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists)

IT \*\*\*251947-22-5P\*\*\* \*\*\*251947-24-7P\*\*\*

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or  
reagent)

(prepn. of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

\*\*\*\*\*

L3 ANSWER 14 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 13 Oct 1999

ACCESSION NUMBER: 1999:650392 HCAPLUS

DOCUMENT NUMBER: 131:271765

TITLE: Preparation of new cephalosporin derivatives as anti-bacterial agents

INVENTOR(S): Takagi, Hiroyasu; Yotsuji, Minako; Kanna, Hiroshi; Matsukura, Hiroko; Murakami, Makoto; Suzuki, Keisuke; Minami, Shinzaburo; Watanabe, Yasuo

PATENT ASSIGNEE(S): Toyama Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 53 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

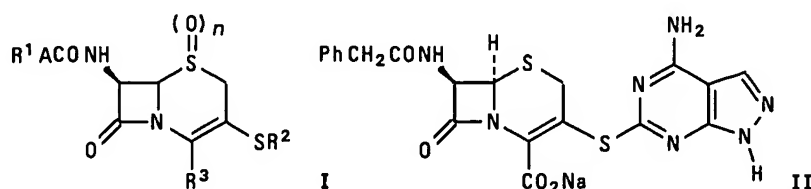
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
JP 11279180	A2	19991012	JP 1999-13670	19990122
PRIORITY APPLN. INFO.:			JP 1998-26582	19980123
			JP 1998-33597	19980130

OTHER SOURCE(S): MARPAT 131:271765

GI



AB Cephalosporin derivs. of formula I [ $R^1$  = H, halo, CN, alkyl, alkoxy, alkylcarbonyloxy, etc.; A =  $\text{CH}_2$ , cycloalkylidene, vinylidene, etc.;  $R^2$  = heteroaryl, etc.;  $R^3$  =  $\text{CO}_2\text{H}$ , carboxylate;  $n$  = 0, 1] are prepd. as antibacterial agents. Thus, 4-aminopyrazolo[3,4-d]pyrimidin-6-ylthiol was added to 7-phenylacetamide-3-trifluorosulfonyloxy-3-cephem-4-carboxylic acid diphenylmethyl ester 1 $\beta$ -oxide, then transformed into II. The MIC value of II against *S. aureus* FDA 209P was 0.2  $\mu\text{g/mL}$ . Pharmaceutical compns. contg. I are described.

IT \*\*\*245487-76-7P\*\*\* \*\*\*245488-78-2P\*\*\* \*\*\*245488-81-7P\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

L3 ANSWER 14 OF 30 HCAPLUS COPYRIGHT 2004 ACS

(prepn. of cephalosporin derivs. as antibacterial agents)

IT \*\*\*245486-48-0P\*\*\* \*\*\*245487-14-3P\*\*\* \*\*\*245488-25-9P\*\*\*

\*\*\*245488-28-2P\*\*\* \*\*\*245488-50-0P\*\*\* \*\*\*245488-54-4P\*\*\*

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of cephalosporin derivs. as antibacterial agents)

\*\*\*\*\*

L3 ANSWER 15 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 09 Sep 1999

ACCESSION NUMBER: 1999:571295 HCAPLUS

DOCUMENT NUMBER: 131:281026

TITLE: Selective A<sub>1</sub>-adenosine receptor antagonists identified using yeast *Saccharomyces cerevisiae* functional assays

AUTHOR(S): Campbell, Robert M.; Cartwright, Craig; Chen, Wei; Chen, Yong; Duzic, Emir; Fu, Jian-Min; Loveland, Michelle; Manning, Ron; McKibben, Bryan; Pleiman, Christopher M.; Silverman, Lauren; Trueheart, Joshua; Webb, David R.; Wilkinson, Vicki; Witter, David J.; Xie, Xiaobing; Castelhana, Arlindo L.

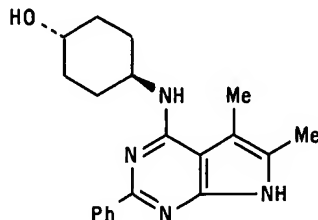
CORPORATE SOURCE: Cadus Pharmaceutical Corporation, Tarrytown, NY, 10591, USA  
SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(16), 2413-2418  
CODEN: BMCLE8; ISSN:0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB Evaluation of a biased "library" of pyrrolo[2,3-d]pyrimidines using yeast-based functional assays expressing human A<sub>1</sub>- and A<sub>2a</sub>-adenosine receptors, led to the A<sub>1</sub> selective antagonist I.

L3 ANSWER 15 OF 30 HCAPLUS COPYRIGHT 2004 ACS

A direct correlation between yeast functional activity and binding data was established. Practical compds. with polar residues at C-4 of the pyrrolopyrimidine system required H-bond donor functionality for high potency.

IT \*\*\*177499-40-0P\*\*\*      \*\*\*246855-41-4P\*\*\*      \*\*\*246855-42-5P\*\*\*  
 \*\*\*246855-43-6P\*\*\*      \*\*\*246855-44-7P\*\*\*      \*\*\*246855-45-8P\*\*\*  
 \*\*\*246855-46-9P\*\*\*      \*\*\*246855-47-0P\*\*\*      \*\*\*246855-48-1P\*\*\*

RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(selective A<sub>1</sub>-adenosine receptor antagonists identified using yeast functional assays)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

\*\*\*\*\*

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE 48

L3 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 07 Jan 1999

ACCESSION NUMBER: 1999:9714 HCAPLUS

DOCUMENT NUMBER: 130:71627

TITLE: Compositions and methods for preventing restenosis following revascularization procedures

INVENTOR(S): Martin, Pauline L.; McAfee, Donald A.

PATENT ASSIGNEE(S): Discovery Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 26 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WD 9857651	A1	19981223	WD 1998-US12717	19980618
W: AU, CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9880740	A1	19990104	AU 1998-80740	19980618
AU 740770	B2	20011115		
EP 1014995	A1	20000705	EP 1998-929099	19980618
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002505687	T2	20020219	JP 1999-504810	19980618
US 6372723	B1	20020416	US 1999-456432	19991208
US 2001009907	A1	20010726	US 2001-783032	20010215
US 6339072	B2	20020115		

PRIORITY APPLN. INFO.:

US 1997-50031P P 19970618

WD 1998-US12717 W 19980618

US 1999-456432 A3 19991208

**AB** In the present invention, a method is provided which reduces or prevents restenosis following revascularization procedures. It has now been found that selective stimulation of adenosine A<sub>2A</sub> receptors can reduce or prevent such restenosis. This method may be achieved either by: (a) the administration of selective adenosine A<sub>2A</sub> receptor agonists, (b) the administration of a selective adenosine A<sub>1</sub> antagonist in combination with either a selective adenosine A<sub>2A</sub> receptor agonist or a non-selective adenosine agonist, or (c) the administration of a selective adenosine A<sub>1</sub> antagonist in order to block adenosine A<sub>1</sub> receptor activation by endogenously-released adenosine. The present invention is also directed to an improved surgical procedure that relies upon selective stimulation of adenosine A<sub>2A</sub> receptors. The degree of arterial stenosis in rabbits after angioplasty treated with the adenosine A<sub>2A</sub> selective agonist 2-cyclohexylmethylenhydrazinoadenosine was significantly less than arterial

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE 49

L3 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 2004 ACS

stenosis in rabbits treated with vehicle.

IT \*\*\*130147-80-7\*\*\*

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(compos. for preventing restenosis following revascularization procedures)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

\*\*\*\*\*

L3 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 27 Apr 1998

ACCESSION NUMBER: 1998:239113 HCAPLUS

DOCUMENT NUMBER: 128:299556

TITLE: Compositions and methods for modulating melanin production

INVENTOR(S): Manneth, Victor; Patel, Rajesh

PATENT ASSIGNEE(S): Therasys, Inc., USA; Manneth, Victor; Patel, Rajesh

SOURCE: PCT Int. Appl., 26 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9815276	A1	19980416	WO 1997-US18148	19971008
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5998423	A	19991207	US 1997-940338	19970930
CA 2242525	AA	19980416	CA 1997-2242525	19971008
AU 9746728	A1	19980505	AU 1997-46728	19971008
EP 880353	A1	19981202	EP 1997-945558	19971008
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
NZ 330862	A	20000728	NZ 1997-330862	19971008
JP 2002515885	T2	20020528	JP 1998-517708	19971008



# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

50

L3 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2004 ACS

PRIORITY APPLN. INFO.:

US 1996-27944P P 19961008

US 1997-940338 A 19970930

WO 1997-US18148 W 19971008

OTHER SOURCE(S): MARPAT 128:299556

AB Compns. and methods for the modulation of melanin prodn. are provided in which the active component is an adenosine receptor antagonist or agonist. A formulation for topical delivery of 8-cyclopentyl-1,3-dimethylxanthine was prepd.

IT \*\*\*206197-05-9\*\*\*

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(compns. for modulating melanin prodn.)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

\*\*\*\*\*

L3 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 31 Jul 1997

ACCESSION NUMBER: 1997:478038 HCAPLUS

DOCUMENT NUMBER: 127:156859

TITLE: Interest of cluster significance analysis in structure-affinity relationships for non-xanthine heterocyclic antagonists of adenosine

AUTHOR(S): Adenot, M.; Benezech, V.; Bompert, J.; Bonnet, P. A.; Chapat, J. P.; Grassy, G.

CORPORATE SOURCE: Centre de Biochimie Structurale, UMR CNRS 9955, INSERM U414, Faculte de Pharmacie, Montpellier, 34060, Fr.

SOURCE: European Journal of Medicinal Chemistry (1997), 32(6), 493-504  
CODEN: EJMCA5; ISSN:0223-5234

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To define some predictive rules for the discrimination of adenosine antagonists by their A<sub>1</sub>-receptor affinity, the authors performed a systematic QSAR anal. As no significant descriptors of affinity were found, the authors then proposed to introduce a calcd. enthalpy or entropy change for the interaction as a first approxn. of the affinity descriptors. Since the structural details of the common receptor binding site remain to be detd., an indirect strategy was utilized involving the simulation of amino acid residues that are thought to interact with the ligand. Estg. enthalpic and entropic components by means of a semi-empirical quantum mech. AM1 force calcn., the authors found a significant clustering of enthalpy change values. This method provides a good descriptor of interaction and also a simple tool for testing hypotheses on the nature of putative binding sites.

IT \*\*\*130147-79-4\*\*\* \*\*\*130147-80-7\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified);  
BIOL (Biological study)

(cluster significance anal. in structure-affinity relationships for non-xanthine heterocyclic antagonists of adenosine)

\*\*\*\*\*

L3 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 12 Sep 1996

ACCESSION NUMBER: 1996:544121 HCAPLUS

DOCUMENT NUMBER: 125:237579

TITLE: New Purines and Purine Analogs as Modulators of Multidrug Resistance

AUTHOR(S): Dhainaut, Alain; Regnier, Gilbert; Tizot, Andre; Pierre, Alain; Leonce, Stephane; Guilbaud, Nicolas; Kraus-Berthier, Laurence; Atassi, Ghanem

CORPORATE SOURCE: Institut de Recherches Servier, Suresnes, 92150, Fr.

SOURCE: Journal of Medicinal Chemistry (1996), 39(20), 4099-4108

CODEN: JMCMAR; ISSN:0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of 36 purine and purine analog derivs. have been synthesized and tested for their ability to modulate multidrug resistance in vitro (P388/VCR-20 and KB-A1 cells) and in vivo (P388/VCR leukemia). Compds. were compared to S9788, a triazine deriv. which has already shown some activity during phase 1 clin. trials and also a limiting cardiovascular side effect possibly linked to its calcium channel affinity. The fact that active compds. increase adriamycin accumulation in the resistant KB-A1 cells, and not in the sensitive KB-3-1 cells, suggests they act predominantly by inhibiting the P-glycoprotein-catalyzed efflux of cytotoxic agents. No direct relation was found between the affinity for the phenylalkylamine binding site of the calcium channel and in vitro sensitization of resistant cells. In vivo, when administered po in assocn. with vincristine (0.25 mg/kg), five of the compds., of very differing calcium channel affinities ( $K_i$  from 5 to 560 nM), fully restored ( $T/V \geq 1.4$ ) the sensitivity of P388/VCR leukemia to vincristine.

IT \*\*\*181862-15-7P\*\*\* \*\*\*181862-16-8P\*\*\*

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of new purines and purine analogs as modulators of multidrug resistance)

IT \*\*\*157838-12-5P\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of new purines and purine analogs as modulators of multidrug resistance)

\*\*\*\*\*

L3 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 23 Jul 1996

ACCESSION NUMBER: 1996:432308 HCAPLUS

DOCUMENT NUMBER: 125:157747

TITLE: Theoretical structure-activity studies of adenosine A<sub>1</sub> ligands: requirements for receptor affinity

AUTHOR(S): Dooley, Michael J.; Kono, Motomichi; Suzuki, Fumio

CORPORATE SOURCE: Pharmaceutical Res. Lab., Kyowa Hakko Kogyo Co. Ltd., Shizuoka-ken, 411, Japan

SOURCE: Bioorganic &amp; Medicinal Chemistry (1996), 4(6), 923-934

CODEN: BMECEP; ISSN:0968-0896

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The three-dimensional (3-D) requirements for A<sub>1</sub> adenosine receptor affinity have been studied based on hydrogen-bonding functionality correlation between a group of twelve A<sub>1</sub> adenosine receptor ligands representing ten structurally different classes of compds. Electrostatic potential similarity indexes and shape similarity indexes strongly support the proposed receptor-bound orientations of the ligands. We conclude, in areas common to both agonist and antagonist binding at the A<sub>1</sub> receptor, that the ligands are recognized by a similar physicochem. 3-D environment. The finding of similar 3-D requirements for agonists and antagonists suggests a fairly static receptor structure in the region common to agonist and antagonist binding. The ribose moiety is remote from antagonist binding site. Such a 3-D environment rationalizes the binding of a no. of potent novel antagonists including KW-3902, not previously reported in modeling studies.

IT \*\*\*130147-80-7\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(theor. structure-activity studies of adenosine A<sub>1</sub> ligands: requirements for receptor affinity)

\*\*\*\*\*

L3 ANSWER 21 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 23 Jul 1996

ACCESSION NUMBER: 1996:432307 HCAPLUS

DOCUMENT NUMBER: 125:157746

TITLE: Conformational search for the N<sup>6</sup>-substituted adenosine analogs and related adenosine A<sub>1</sub> receptor antagonists

AUTHOR(S): Dooley, Michael L.; Kono, Motomichi; Suzuki, Fumio

CORPORATE SOURCE: Pharmaceutical Res. Lab., Kyowa Hakko Kogyo Co. Ltd., Shizuoka-ken, 411, Japan

SOURCE: Bioorganic &amp; Medicinal Chemistry (1996), 4(6), 917-921

CODEN: BMECEP; ISSN:0968-0896

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The search for 3-D requirements for the adenosine A<sub>1</sub> receptor affinity is useful to aid in the design of more potent and/or novel ligands as pharmacol. tools and therapeutics for the receptor. To emboss 3-D requirements for adenosine A<sub>1</sub> receptor affinity among adenosine receptor antagonists, adenosine and xanthine analogs, conformations for the N<sup>6</sup>-substituted adenosine analogs and related adenosine A<sub>1</sub> receptor antagonists were thoroughly searched by semi-empirical quantum mechanics calcns. Newly established global min. for these compds. (C1'-N<sup>6</sup>-C6-N1 torsion: 10°) are consistent with retrieved structures from Cambridge Structural Database and previously published NMR data on the soln. conformation of N<sup>6</sup>-substituted adenosine analogs. However, these newly studied global min. for adenosine analogs are different from those previously reported (C1'-N<sup>6</sup>-C6-N1 torsion: ±75°).

IT \*\*\*130147-80-7\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(conformational search for the N<sup>6</sup>-substituted adenosine analogs and related adenosine A<sub>1</sub> receptor antagonists)

\*\*\*\*\*

L3 ANSWER 22 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 06 Jun 1996

ACCESSION NUMBER: 1996:328283 HCAPLUS

DOCUMENT NUMBER: 125:25634

TITLE: Chiral Pyrrolo[2,3-d]pyrimidine and Pyrimido[4,5-b]indole Derivatives:  
Structure-Activity Relationships of Potent, Highly Stereoselective  
A<sub>1</sub>-Adenosine Receptor Antagonists

AUTHOR(S): Mueller, Christa E.; Geis, Uli; Grahner, Bettina; Lanzner, Wolfgang;  
Eger, Kurt

CORPORATE SOURCE: Institut fuer Pharmazie und Lebensmittelchemie Pharmazeutische  
Chemie, Julius-Maximilians-Universitaet, Wuerzburg, D-97074, Germany

SOURCE: Journal of Medicinal Chemistry (1996), 39(13), 2482-2491

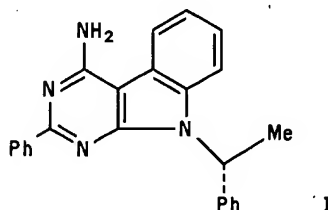
CODEN: JMCMAR; ISSN:0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB A series of novel, mostly chiral pyrrolo[2,3-d]pyrimidine and pyrimido[4,5-b]indole derivs. has been synthesized and investigated in radioligand binding assays at the high-affinity adenosine receptor (AR) subtypes A<sub>1</sub> and A<sub>2a</sub>. The compds. can be envisaged as adenine and hypoxanthine analogs lacking the nitrogen in the 7-position (7-deazaadenines and 7-deazahypoxanthines). 7-Deazaadenines were much more potent than 7-deazahypoxanthines at AR with A<sub>1</sub>AR affinities in the low-nanomolar range, extraordinarily high selectivity for the rat brain A<sub>1</sub>AR vs. the A<sub>2a</sub>AR (several thousand-fold), and high stereoselectivity (up to 96-fold). Pyrimido[4,5-b]indoles were more potent A<sub>1</sub>AR antagonists compared to pyrrolo[2,3-d]pyrimidines. Compd. I is one of the most potent and most selective nonxanthine A<sub>1</sub>AR antagonists known to date (K<sub>i</sub> = 2.8 nM, >2000-fold A<sub>1</sub>-selective). A new class of very potent A<sub>1</sub>AR antagonists has been identified, namely, 2-phenyl-7-deazaadenines bearing a substituent at the exocyclic amino group (N<sup>4</sup>-substituted 2-phenyl-7-deazaadenines).

(R)-N-(1-Phenylethyl)-4-amino-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine (DPEAP) showed a K<sub>i</sub> value of 6.7 nM at A<sub>1</sub>AR and >4000-fold A<sub>1</sub> selectivity. Different binding modes are

## L3 ANSWER 22 OF 30 HCAPLUS COPYRIGHT 2004 ACS

postulated for the N<sup>4</sup>-substituted 4-aminopyrrolo[2,3-d]pyrimidines and the 7-substituted derivs., based on a comparison of steric, electronic, and hydrophobic properties of the two classes of compds. Water soly. and lipophilicity have been detd. for selected compds.

4-Amino-5,6-dimethyl-2-(3-chlorophenyl)-7H-pyrrolo[2,3-d]pyrimidine showed the highest water soly./A<sub>1</sub>AR affinity ratio of 368 in the present series, over 2000-fold A<sub>1</sub> selectivity, and 64-fold stereoselectivity (R > S).

IT	***130147-80-7P***	***130147-81-8P***	***177499-32-0P***
	***177499-33-1P***	***177499-34-2P***	***177499-35-3P***
	***177499-36-4P***	***177499-37-5P***	***177499-40-0P***
	***177499-41-1P***	***177570-32-0P***	***177570-33-1P***
	***177570-34-2P***	***177570-35-3P***	

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified);  
SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(prepn. and structure-activity of pyrroloindoles and pyrrolopyrimidines as A<sub>1</sub>-adenosine  
receptor antagonists)

\*\*\*\*\*

L3 ANSWER 23 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 21 Feb 1996

ACCESSION NUMBER: 1996:109105 HCAPLUS

DOCUMENT NUMBER: 124:249637

TITLE: A survey of nonxanthine derivatives as adenosine receptor ligands  
AUTHOR(S): Siddiqi, Suhaib M.; Ji, Xiao-duo; Melman, Neli; Olah, Mark E.; Jain, Rahul; Evans, Patricia; Glashofer, Marc; Padgett, William L.; Cohen, Louis A.; et al.

CORPORATE SOURCE: Molecular Recognition Section, National Institutes of Health, Bethesda, MD, 20892, USA

SOURCE: Nucleosides & Nucleotides (1996), 15(1-3), 693-717  
CODEN: NUNUD5; ISSN:0732-8311

PUBLISHER: Dekker

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The binding affinities at rat A<sub>1</sub>, A<sub>2a</sub>, and A<sub>3</sub> adenosine receptors of a wide range of heterocyclic derivs. have been detd. Mono-, bi-, tricyclic and macrocyclic compds. were screened in binding assays, using either [<sup>3</sup>H]PIA or [<sup>3</sup>H]CGS 21680 in rat brain membranes or [<sup>125</sup>I]AB-MECA in CHO cells stably transfected with rat A<sub>3</sub> receptors. Several new classes of adenosine antagonists (e.g. 5-oxoimidazopyrimidines and a pyrazoloquinazoline) were identified. Various sulfonylpiperazines, 11-hydroxytetrahydrocarbazolenine, 4H-pyrido[1,2-a]pyrimidinone, folic acid, and cytochalasin H and J bound to A<sub>3</sub> receptors selectively. Moreover, cytochalasin A, which bound to A<sub>1</sub> adenosine receptors with K<sub>i</sub> value of 1.9 μM, inhibited adenylyl cyclase in rat adipocytes, but not via reversible A<sub>1</sub> receptor binding.

IT \*\*\*111601-39-9\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(nonxanthine derivs. as adenosine receptor ligands)

\*\*\*\*\*



L3 ANSWER 24 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 05 Oct 1995

ACCESSION NUMBER: 1995:833632 HCAPLUS

DOCUMENT NUMBER: 123:313913

TITLE: A One-Step Ring Transformation/Ring Annulation Approach to  
Pyrrolo[2,3-d]pyrimidines. A New Synthesis of the Potent  
Dihydrofolate Reductase Inhibitor TNP-351

AUTHOR(S): Taylor, Edward C.; Patel, Hemantkumar H.; Jun, Jong-Gab

CORPORATE SOURCE: Department of Chemistry, Princeton University, Princeton, NJ, 08544,  
USA

SOURCE: Journal of Organic Chemistry (1995), 60(21), 6684-7  
CODEN: JOCEAH; ISSN:0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:313913

AB Condensation of amidines with 2-amino-3-cyanofurans gives  
2-substituted-4-aminopyrrolo[2,3-d]pyrimidines by a ring-opening, ring-recyclization sequence of  
reactions through which the starting furan 2-amino nitrogen becomes the pyrrole nitrogen of  
the final product and one of the amidine nitrogens becomes N-1 of the fused pyrimidine  
ring. 2,4-Diamino-5-[2-(4-carbethoxyphenyl)ethyl]pyrrolo[2,3-d]pyrimidine, a key intermediate in  
the synthesis of the dihydrofolate reductase inhibitor TNP-351, has been prepd. in one step  
by reaction of 4-[2-(2-amino-3-cyano-4-furanyl)ethyl]benzoic acid Et ester with guanidine.

IT \*\*\*170170-17-9P\*\*\*

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of pyrrolo[2,3-d]pyrimidines from guanidines and (amino)furan carbonitriles)

\*\*\*\*\*

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE 59

L3 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 29 Oct 1994

ACCESSION NUMBER: 1994:605381 HCAPLUS

DOCUMENT NUMBER: 121:205381

TITLE: Preparation of purine derivatives and analogs as agents for suppressing tumor cell resistance to antineoplastic agents

INVENTOR(S): Regnier, Gilbert; Dhainaut, Alain; Atassi, Ghanem; Pierre, Alain

PATENT ASSIGNEE(S): Adir et Compagnie, Fr.

SOURCE: PCT Int. Appl., 30 pp

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

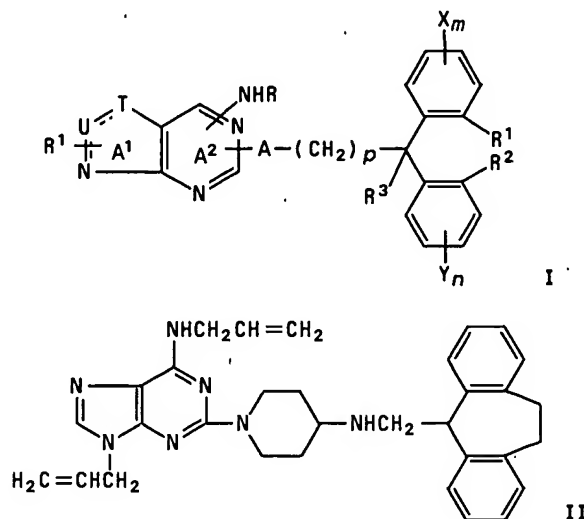
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
WO 9413668	A1	19940623	WO 1993-FR1211	19931209
W: AU, CA, JP, NZ, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
FR 2699176	A1	19940617	FR 1992-14913	19921211
FR 2699176	B1	19950303		
CA 2117462	AA	19940623	CA 1993-2117462	19931209
AU 9456535	A1	19940704	AU 1994-56535	19931209
AU 666422	B2	19960208		
EP 673376	A1	19950927	EP 1994-902003	19931209
EP 673376	B1	19960522		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 08504426	T2	19960514	JP 1993-513866	19931209
AT 138380	E	19960615	AT 1994-902003	19931209
ES 2091126	T3	19961016	ES 1994-902003	19931209
US 5508277	A	19960416	US 1994-284689	19940810
PRIORITY APPLN. INFO.:				
			FR 1992-14913	19921211
			WO 1993-FR1211	19931209

OTHER SOURCE(S): MARPAT 121:205381

GI

L3 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 2004 ACS



AB The title compds. I [T and U represent CH or N, and rings  $A^1$  and  $A^2$  together form purine ring, pyrazolo[3,4-d]pyrimidine, etc.; R,  $R'$  = alkyl, alkenyl; A = heteromonocyclic moiety (further details on said heteromonocyclic moiety are given); p = 0 or 1; X, Y = H, halo, etc.; m, n = 1 - 3;  $R^1$ ,  $R^2$  = H, alkyl; or  $R^1R^2$  = O,  $(CH_2)_x$ , etc; x = 1 - 3;  $R^3$  = H, Ph] are prepd. Purine deriv. II was prepd. from 2,6-dichloropurine in multiple steps. Mice with transplanted tumor were dosed with II (25 mg/Kg i.p.) and vincristine (0.50 mg/kg i.p.). The survival time of said mice was 1.54 times survival time of mice with tumor receiving vincristine therapy.

IT \*\*\*157838-12-5P\*\*\*

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, as agent for suppressing tumor cell resistance to antineoplastic agents)

\*\*\*\*\*

L3 ANSWER 26 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 08 Dec 1990

ACCESSION NUMBER: 1990:611696 HCAPLUS

DOCUMENT NUMBER: 113:211696

TITLE: 7-Deaza-2-phenyladenines: structure-activity relationships of potent A<sub>1</sub> selective adenosine receptor antagonists

AUTHOR(S): Mueller, Christa E.; Hide, Izumi; Daly, John W.; Rothenhaeusler, Klaus; Eger, Kurt

CORPORATE SOURCE: Lab. Bioorg. Chem., Natl. Inst. Diabetes, Dig. Kidney Dis., Bethesda, MD, 20892, USA

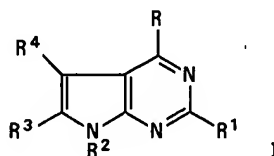
SOURCE: Journal of Medicinal Chemistry (1990), 33(10), 2822-8  
CODEN: JMCMAR; ISSN:0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:211696

GI



AB 7-Deazapurines I [R = NH<sub>2</sub>, Cl, OH, SH, SMe, SO<sub>2</sub>Me; R<sup>1</sup> = H, SH, SMe, SO<sub>2</sub>Me, Me, Ph, 4-ClC<sub>6</sub>H<sub>4</sub>; R<sup>2</sup> = H, Ph, hexyl, allyl, 2,3-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 4-BrC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, 2-deoxyribosyl, CHMePh; R<sup>3</sup> = R<sup>4</sup> = Me, H, CHO, CO<sub>2</sub>H; R<sup>3</sup>R<sup>4</sup> = (CH<sub>2</sub>)<sub>4</sub>, CH:CHCH:CH] were prepd. in an attempt to improve the adenosine receptor affinity and A<sub>1</sub> or A<sub>2</sub> selectivity. The adenosine receptor affinities were assessed by measuring the inhibition of [<sup>3</sup>H]-(R)-N-(phenylisopropyl)adenosine (II) binding to rat brain A<sub>1</sub> and inhibition of [<sup>3</sup>H]-5'-(N-ethylcarboxamido)adenosine (III) binding to rat striatum A<sub>2</sub> adenosine receptors. Selected I were further examd. in adenosine receptor coupled adenylate cyclase assays. All tested compds. antagonized the inhibition of adenylate cyclase elicited by interaction of II with A<sub>1</sub> receptors in rat fat cell membranes and the activation of adenylate cyclase elicited by interaction of III with A<sub>2</sub> receptors of pheochromocytoma PC12 cell membranes. The results indicate that 7-deazahypoxanthines have a potential for A<sub>2</sub> selectivity, while all 7-deazaadenines are A<sub>1</sub> selective. Introduction of a Ph residue in the 2-position of 7-deazaadenines increases A<sub>1</sub> activity tremendously. Thus, I (R = NH<sub>2</sub>, R = 4-ClC<sub>6</sub>H<sub>4</sub>, R<sup>2</sup> = Ph, R<sup>3</sup> = R<sup>4</sup> = Me) is potent and specific for the A<sub>1</sub> receptors of rat brain (K<sub>i</sub> = 122 nM), having no affinity for the A<sub>2</sub> receptors of rat striatum. The compd. has low activity at the A<sub>2</sub> receptors of rat PC12 cell membranes where it appears to act as a noncompetitive inhibitor. The most potent A<sub>1</sub> antagonist was I [R = NH<sub>2</sub>, R<sup>1</sup> = Ph, R<sup>2</sup> = (R)-CHMePh, R<sup>3</sup> = R<sup>4</sup> = Me].

L3 ANSWER 26 OF 30 HCAPLUS COPYRIGHT 2004 ACS

IT \*\*\*111601-39-9\*\*\* \*\*\*111601-40-2\*\*\* \*\*\*130147-78-3\*\*\*  
\*\*\*130147-79-4\*\*\* \*\*\*130147-80-7\*\*\* \*\*\*130147-81-8\*\*\*  
\*\*\*130147-82-9\*\*\* \*\*\*130147-83-0\*\*\*

RL: RCT (Reactant); RACT (Reactant or reagent)  
(adenosine receptor antagonist activity of)

\*\*\*\*\*

L3 ANSWER 27 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 28 Oct 1988

ACCESSION NUMBER: 1988:549471 HCAPLUS

DOCUMENT NUMBER: 109:149471

TITLE: Phosphorus pentoxide in organic synthesis. XXXVI. Synthesis of  
7H-pyrrolo[2,3-d]pyrimidine-2,4-diamines and 7-diazaisoguanines from  
7H-pyrrolo[2,3-d]pyrimidine-2,4-diones

AUTHOR(S): Joergensen, Anker; Moharram, H. H.; Pedersen, Erik B.

CORPORATE SOURCE: Dep. Chem., Odense Univ., Odense, DK-5230, Den.

SOURCE: Chemica Scripta (1988), 28(2), 201-4

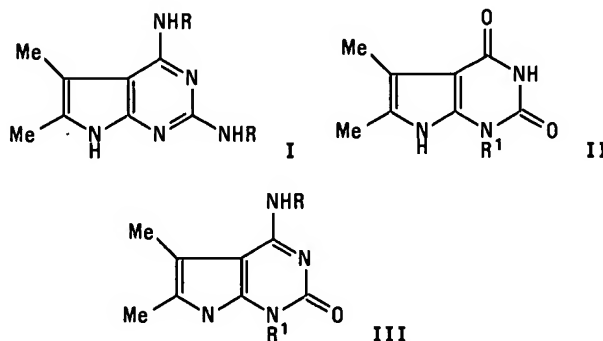
CODEN: CSRPB9; ISSN:0004-2056

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:149471

GI



AB Diaryldimethylpyrrolopyrimidinediamines I (R = Ph, *m*-tolyl, *p*-tolyl, C<sub>6</sub>H<sub>4</sub>Bu-*p*, 3,5-xylyl) were prepd. in ca. 20% yield by heating dimethylpyrrolopyrimidinedione II (R<sup>1</sup> = H) with a mixt. of P<sub>2</sub>O<sub>5</sub>, Et<sub>3</sub>N.HCl, and RNH<sub>2</sub> in a 1:4:4 molar ratio. Under similar reaction conditions II (R<sup>1</sup> = Me) afforded 40-50% (arylamino)pyrrolopyrimidinones III (R<sup>1</sup> = Me). The reaction of 1 equiv II (R<sup>1</sup> = H) with 8 equiv P<sub>2</sub>O<sub>5</sub>, Et<sub>3</sub>N.HCl, and RNH<sub>2</sub> gave 35-54% III (R<sup>1</sup> = H).

L3 ANSWER 27 OF 30 HCAPLUS COPYRIGHT 2004 ACS

IT \*\*\*116673-05-3P\*\*\* \*\*\*116673-06-4P\*\*\* \*\*\*116673-07-5P\*\*\*

\*\*\*116673-08-6P\*\*\* \*\*\*116673-09-7P\*\*\*

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

\*\*\*\*\*

L3 ANSWER 28 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 25 Dec 1987

ACCESSION NUMBER: 1987:636656 HCAPLUS

DOCUMENT NUMBER: 107:236656

TITLE: Selected reactions on the o-aminonitrile system of substituted pyrroles

AUTHOR(S): Eger, Kurt; Pfahl, Johannes Georg; Folkers, Gerd; Roth, Hermann J.

CORPORATE SOURCE: Pharm. Inst., Univ. Tuebingen, Tuebingen, D-7400, Fed. Rep. Ger.

SOURCE: Journal of Heterocyclic Chemistry (1987), 24(2), 425-30

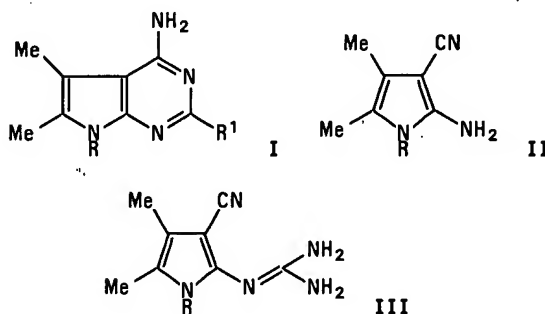
CODEN: JHTCAD; ISSN:0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 107:236656

GI



AB Pyrrolo[2,3-d]pyrimidine-2,4-diamines I (R = Ph, PhCHMe, R<sup>1</sup> = NH<sub>2</sub>) were prepd. from pyrroles II via amidines III. I (R = Ph, PhCHMe, R<sup>1</sup> = Me, Ph, *p*-ClC<sub>6</sub>H<sub>4</sub>) were prepd. from II and R<sup>1</sup>CN. Some unexpected reactions on the 2-aminopyrrole-3-carbonitrile system are described.

IT \*\*\*111601-36-6P\*\*\* \*\*\*111601-37-7P\*\*\*

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and deprotection of, with polyphosphoric acid)

# STN INTERNATIONAL®

HCAPLUS FILE SEARCH RESULTS - P077139C

17 MAR 2004 20:04:19

PAGE

64

L3 ANSWER 28 OF 30 HCAPLUS COPYRIGHT 2004 ACS

IT \*\*\*111601-39-9P\*\*\* \*\*\*111601-40-2P\*\*\*

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

\*\*\*\*\*

L3 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 22 Apr 2001

ACCESSION NUMBER: 1962:476026 HCAPLUS

DOCUMENT NUMBER: 57:76026

ORIGINAL REFERENCE NO.: 57:15129f-i,15130a-i

TITLE: Pyrrolopyrimidine vasodilators

INVENTOR(S): Hitchings, George H.; Ledig, Kurt W.; West, Robert A.

PATENT ASSIGNEE(S): Burroughs Wellcome & Co. (U.S.A.) Inc.

SOURCE: 5 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	---	-----	-----	-----
US 3037980		19620605	US	
PRIORITY APPLN. INFO.:			GB	19550818

GI For diagram(s), see printed CA Issue.

AB Pyrrolo[2,3-d]pyrimidines, having the structure I, were prepd. usually by reaction of the 4-chloro deriv. with the proper amine. 4-Chloropyrrolo [2,3-d]pyrimidine (II) (1.3 g.), 30 cc. EtOH, 1 drop concd. HCl, and 2.5 cc. PrNH<sub>2</sub> was heated 7 hrs. at 125°, cooled, evapd., and the residue triturated with 5 cc. 2.5% NaOH and filtered to give 1.2 g. I (R<sup>1</sup>, R<sup>2</sup>, R<sup>3</sup> = H, R<sup>4</sup> = Pr), m. 162° (30% aq. EtOH). The following I were prepd. similarly using the proper starting materials (R<sup>1</sup>, R<sup>2</sup>, R<sup>3</sup>, R<sup>4</sup>, and m.p. given): H, Me, H, pentyl, 167-9° (25% EtOH); Me, H, H, pentyl, 125-7° (C<sub>6</sub>H<sub>6</sub>-hexane); H, H, H, Me, 236°; H, H, Me, Me, 222°; H, H, Et, H, 205°; H, H, Et, Me, 170°; H, H, H, pentyl, 129°; H, H, H, CHMe<sub>2</sub>, 169-70°; H, H, Me, Pr, 148-9°; H, H, H, CH<sub>2</sub>CH<sub>2</sub>OH, 209°; H, H, H, CH<sub>2</sub>CH(OEt)<sub>2</sub>, 124-6°; H, H, H, Bu, 145-6°; H, H, H, CH<sub>2</sub>CHMe<sub>2</sub>, 173-4°; H, H, H, CHMeEt, 125-6°; H, H, H, CMe<sub>3</sub>, 183°; H, H, H, CH<sub>2</sub>CH<sub>2</sub>CHMe<sub>2</sub>, 166-7°; H, H, H, CH<sub>2</sub>CHMeEt, 140-1°; H, H, H, hexyl, 150-1°; H, H, H, heptyl, 126-7° [135° (heptane)]; H, H, H, octyl, 118-19°; H, H, H, allyl, 167°; H, H, H, CH<sub>2</sub>CH<sub>2</sub>NHEt, 146-7°; H, H, H, cyclopentyl, 162-3°; H, H, H, CH<sub>2</sub>CH<sub>2</sub>OMe, 167-8°; H, Me, H, CH<sub>2</sub>CH<sub>2</sub>OMe, 144-6°; H, H, H, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OMe, 144-5°; H, H, Me, CHMe<sub>2</sub>, 156-7°; H, H, Et, Et, 174-5°; H, H, Pr, Pr, 118°; H, H, H, piperidino, 184-5°; H, Me, H, Et, 189-90°; Me, H, H, Et, 159°; H, H, Me, pentyl, 133-5°. Reactions of this type with higher mol. wt. amines were carried out by refluxing in an aq. system. For example, 1.2 g. II, 5 g. nonylamine,

## L3 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 2004 ACS

and 50 cc. H<sub>2</sub>O was refluxed 2 hrs., 4 cc. 5% NaOH added, chilled, and filtered to give 2.5 g. I (R<sup>1</sup>, R<sup>2</sup>, R<sup>3</sup> = H, R<sup>4</sup> = nonyl), hemihydrate m. 122-4° (aq. EtOH). The following compds. were prepd. similarly from the appropriate starting materials (R<sup>1</sup>, R<sup>2</sup>, R<sup>3</sup>, R<sup>4</sup>, m.p. given): H, Me, H, benzyl, 205-7°; H, Me, H, N-methylpiperazino, 191-2° (heptane); H, H, H, N'-ethylpiperazino, 175°; H, H, H, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CHMe<sub>2</sub>, 129-30°; H, Ph, H, nonyl, 126-38°; H, H, H, decyl, 110-11°; H, H, H, cyclohexyl, 149-51°; H, H, H, benzyl, 196°; H, Me, H, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-4, 211°; H, H, H, CH<sub>2</sub>CH<sub>2</sub>Ph, 197-8° (HCl salt m. 231-4°); H, H, H, CH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, 164-5°; H, H, H, CH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, 146-7°; H, Me, H, CH<sub>2</sub>CH(OEt)<sub>2</sub>, 129-30°; H, H, H, CH<sub>2</sub>CH<sub>2</sub>CH(OEt)<sub>2</sub>, 120-1°; H, H, H, CO<sub>2</sub>Me, decompd. 265-70°; H, H, H, furyl, 154°; H, H, Me, CH<sub>2</sub>CH(OEt)<sub>2</sub>, 127-9°; H, Me, Me, CH<sub>2</sub>CH(OEt)<sub>2</sub>, 155°; H, H, Me, CH<sub>2</sub>CH<sub>2</sub>CH(OEt)<sub>2</sub>, 87-9°; H, H, Et, CO<sub>2</sub>Me, 204°; H, H, H, morpholino, 215°; H, Me, H, nonyl, 110-13°; H, Me, H, CH<sub>2</sub>CH<sub>2</sub>Ph, 208-9°. In another example 1.7 g. I, 3 g. pyrrolidine, and 35 cc. 95% EtOH were heated in a bomb at 130° 6.5 hrs., evapd., the residue dissolved in H<sub>2</sub>O at pH 2 by adding 1:1 HCl, filtered from tar, adjusted to pH 10 and filtered to give 1.7 g. I (R<sup>1</sup>, R<sup>2</sup>, R<sup>3</sup> = H, R<sup>4</sup> = pyrrolidino), m. 263-5°. The following compds. were prepd. similarly (R<sup>1</sup>, R<sup>2</sup>, R<sup>3</sup>, R<sup>4</sup>, and m.p. given): H, H, H, H, 2905°; H, Me, H, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OMe, 188-9°; H, Me, H, 2-pyridylmethyl, 215-16°; H, Me, H, 3,4,5-trimethoxybenzyl, 216-17°; H, Me, H, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-3, 184-5° (HCl salt m. 230-6°); H, H, H, 2-thenyl, 272-6°; H, H, H, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Cl-2, 220-2°; H, H, H, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-4, 203-5°; H, H, Me, benzyl, 228-30°; H, H, H, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Cl-4, 205-6°; H, H, H, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>OMe-4, 236-9°; H, H, Me, nonyl, 105-6°; H, H, Me, benzyl, 178-80°; H, H, H, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-2, 259-61°; H, H, H, 2-pyridyl, 184-6°; H, H, CH<sub>2</sub>CH<sub>2</sub>OH, CH<sub>2</sub>CH<sub>2</sub>OH, 196-8°; H, Pr, H, nonyl, 94-6°; Me, H, H, nonyl, West-(HCl salt m. 129-30°); Me, Me, H, benzyl, 147-8°; Me, H, H, 4-methylpiperazino, decompd. 190-210° then m. 233-8°; H, Pr, H, benzyl, 161-2°; H, Pr, H, 4-ethylpiperazino, 121°; H, H, H, 4-isopropylpiperazino, 178-9°; H, H, H, 4-propylpiperazino, 172-4°; H, H, H, 4-carbethoxypiperazino, 204-5°; H, H, H, 4-(2hydroxyethyl)piperazino, 176-7°; H, H, H, 4-butylpiperazino, 171-2°; H, H, H, 3,4,5-trimethylpiperazino, 206-7°; H, H, H, 4-ethylpiperazino, 225-30°; H, Me, H, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>OMe-4, 189-91°; H, Me, H, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OCH-Me<sub>2</sub>, 130-40°; H, Me, Me, Pr, 123-4°; H, Me, H, 4-propylpiperazino, 194-6°; H, Me, H, PhCH<sub>2</sub>CH<sub>2</sub>, 208-9° (HCl salt m. 112-16°); H, Me, H, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Cl-4, 234-5°; H, Me, Me, CH<sub>2</sub>Ph, 218-19°; H, Me, H, 2-thenyl, 214-15°; H, Me, H, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Cl-2, 219-22°; H, Me, H, α-furyl, 195-7°. Other pyrrolo[2,3-d]pyrimidines prepd. were (substituents and m.p. given): 4-octyloxy, 107-9°; 4-octylthio, 111-12°; 2,4-Me(Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>O), 201-3°; and 2-methyl, 179-80°. The products have hypotensive, muscle relaxant, hypnotic, and anticonvulsant effects. They are toxic at approx. 100 mg./kg. In dogs at 0.5 to 4 mg./kg. they produce a systolic drop of 5-45 mm. lasting up to 1.5 hrs. EtO<sub>2</sub>CCH(CN)CH<sub>2</sub>CH(OEt)<sub>2</sub> (11.4 g.) in 25 cc. EtOH was mixed with 4.3 g. MeC(NH<sub>2</sub>):NH<sub>2</sub>HCl and 1.15 g. Na in 25 cc. EtOH, refluxed 6 hrs., evapd., adjusted to pH 5 with AcOH and filtered to give an intermediate which in 100 cc. EtOH and 2 cc. concd. H<sub>2</sub>SO<sub>4</sub> was refluxed 6 hrs., cooled, and filtered to give 4-hydroxy-2-methylpyrrolo[2,3-d]pyrimidine. To 5.8 g. II in 40 cc. NaH-dried HCONMe<sub>2</sub> at



L3 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 2004 ACS

15° was added 0.95 g. NaH, the reaction mixt. held at room temp. 6-7 hrs., cooled to 5°, and 6.2 g. MeI added. After 24 hrs. at room temp. and 3-4 hrs. at 45°, 40 cc. H<sub>2</sub>O was added and the reaction mixt. cooled overnight and filtered to give 4.1 g. 7-methyl-4-chloropyrrolo[2,3-d]pyrimidine.

IT \*\*\*94966-89-9\*\*\* , 7H-Pyrrolo[2,3-d]pyrimidine, 4-(nonylamino)-2-phenyl-  
(prepn. of)

\*\*\*\*\*

L3 ANSWER 30 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 22 Apr 2001

ACCESSION NUMBER: 1962:46024 HCAPLUS

DOCUMENT NUMBER: 56:46024

ORIGINAL REFERENCE NO.: 56:8712e-i,8713a-c

TITLE: 2-Alkyl(aryl)- and 2,7-dimethyl-4-substituted  
amino-pyrrolo[2,3-d]pyrimidines

AUTHOR(S): West, R. A.; Beauchamp, L.

CORPORATE SOURCE: Wellcome Research Labs., Tuckahoe, NY

SOURCE: Journal of Organic Chemistry (1961), 26, 3809-12

CODEN: JOCEAH; ISSN:0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 56:46024

AB Amidines condensed with Et  $\alpha$ -cyano- $\gamma,\gamma$ -diethoxybutyrate (I) gave pyrimidine derivs. which were further cyclized to 4-hydroxypyrrolo[2,3-d]pyrimidines. The various 4-chloropyrrolopyrimidines resulting from treatment of the OH compds, with PCl<sub>3</sub> reacted readily with amines to yield 4-substituted amino derivs. having pharmacol. activity. Acetamidine-HCl (4.7 g.) left 1 hr. at room temp. with 75 ml. soln. of 0.1 mole NaOEt, the NaCl removed, the filtrate refluxed 5 hrs. with I, evapd., the residue dissolved in 80 ml. cold H<sub>2</sub>O, the pyrimidine pptd. at pH 7, cooled overnight, and dried gave 10.8 g. 2-methyl-4-hydroxy-5-( $\beta,\beta$ -diethoxyethyl)pyrimidine (II), decompd. at 253-60° to a dark oil. The following 4-hydroxy-6-amino-5-( $\beta,\beta$ -diethoxyethyl)pyrimidines were thus obtained (2-substituent, % yield, m.p. given): Me, 89, 249-50°; Et, 93, 238-5°; Pr, 77, 207-9°; Ph, 71, 174-6°. II (4.5 g.) refluxed 2 hrs. with 2 ml. concd. H<sub>2</sub>SO<sub>4</sub> in 110 ml. 95% alc., an equal vol. of H<sub>2</sub>O added, and the mixt. chilled overnight gave 2.1 g. 2-methyl-4-hydroxypyrrolo[2,3-d]pyrimidine (III), no m.p. below 300°. III (25 g.) suspended in 175 ml. POCl<sub>3</sub> refluxed 45 min., excess POCl<sub>3</sub> evapd. at 55-60° in vacuo, the oil dropped slowly into 1l. ice H<sub>2</sub>O, the product extd. with Et<sub>2</sub>O, dried, and evapd. gave 23.2 g. 2-methyl-4-chloropyrrolo[2,3-d]pyrimidine (IV). IV (5 g.) added to 1.9 g. Na-OMe in 50 ml. alc. at 5-10°, to this added 2.4 ml. MeI, the mixt. warmed 2 days at 40-5° in a sealed flask, the solvent evapd., the solid triturated with H<sub>2</sub>O, and filtered gave 4 g.

## L3 ANSWER 30 OF 30 HCAPLUS COPYRIGHT 2004 ACS

2,7-dimethyl-4-chloropyrrolo[2,3-d]pyrimidine. The following pyrrolo[2,3-d]pyrimidines were thus obtained (2, 7, 4 substituents, % yield, and m.p. given): Me, H, OH, 76, no m.p. to 320°; Et, H, OH, 85, no m.p. to 320°; Pr, H, OH, 85, no m.p. to 320°; Ph, H, OH, 93, no m.p. to 320°; H, Me, Cl, 75, 130°; Me, H, Cl, 83, 205-7°; Me, Me, Cl, 70, 121-2°; Et, H, Cl, 72, 125-7°; Pr, H, Cl, 82, 129-30°; Ph, H, Cl, 80, 225-6°. Method A.

2-Phenyl-4-chloropyrrolo[2,3-d]pyrimidine (1 g.) added to 35 ml. H<sub>2</sub>O contg. 0.9 g. K<sub>2</sub>CO<sub>3</sub> and 1 g. PhCH<sub>2</sub>NH<sub>2</sub> and cooled overnight gave 1.2 g. crude

2-phenyl-4-benzylaminopyrrolo[2,5-d]pyrimidine. The product was recrystd. from C<sub>6</sub>H<sub>6</sub>heptane. Method B. IV (2.06 g.) and 6.04 g. o-anisidine refluxed 1.5 hrs. with 17 ml. HCONMe<sub>2</sub>, chilled overnight with an equal vol. of H<sub>2</sub>O, filtered, and dried gave 3.1 g.

2-methyl-4-(2-methoxyanilino)pyrrolo[2,3-d]pyrimidine, m. 255-6° (decompn.). IV (2 g.) suspended in 40 ml. concd. NH<sub>4</sub>OH heated 4.5 hrs. at 145° in a bomb, evapd., and the product collected gave 1.3 g. 2-methyl-4-aminopyrrolo[2,3-d]pyrimidine, m. 305-7° (decompn.).

The following 4substituted aminopyrrolo[2,3-d]pyrimidines were thus obtained (2, 7, 3 substituents, m.p., and % yield given): H, Me, NH<sub>4</sub>Et, 157-8°, 88; Me, H, NH<sub>4</sub>Et, 189-90°, 89; Me, H, CMePr, 124-5°, 93; Me, H, 2-thenylamino, 214-15°, 91; Me, H, NHC<sub>6</sub>H<sub>4</sub>Me-m, 248°, 98; Me, Me, NHCH<sub>2</sub>Ph, 147-8°, 90; Me, H, NHCH<sub>2</sub>Ph, 223-4°, 93; Et, H, NHCH<sub>2</sub>Ph, 183°, 90; Pr, H, NHCH<sub>2</sub>Ph, 170-1°, 92; Ph, H, NHCH<sub>2</sub>Ph, 162-4°, 92. The ultraviolet spectral data of pyrrolo[2,3-d]pyrimidines and precursors were given in a table at pH 1.0 and pH 11.0. Some of the substituted amino compds, had pronounced pharmacol. effects in test animals including anticonvulsant, muscle relaxant, hypotensive and tranquilizer activities.

IT \*\*\*94304-61-7\*\*\* , 7H-Pyrrolo[2,3-d]pyrimidine, 4-(benzylamino)-2-phenyl-  
(prepn. of)

IT \*\*\*92193-06-1\*\*\* , 7H-Pyrrolo[2,3-d]pyrimidine, 4-(ethylamino)-2-phenyl-  
(spectrum of)

\*\*\*\*\*